

FORMAL MODELING

Algebra and Logic in Mathematical Modeling



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1. Introduction

2. Symbolic Summation and the Modeling of Sequences

3. Logical Models of Problems and Computations

4. Modeling Problems in Geometry and Discrete Mathematics

- Problem 1: How to get from A to B ?
- Problem 2: How to efficiently use resources?

5. Organization

Introduction

What is this course about?

- Application of techniques from symbolic computation.
 - Rooted in computer algebra, algebraic geometry, computational logic.
 - Focus is on correct formalization, precise analysis, exact solving (rather than on fast but numerically approximated computations).
- Modeling and analysis of problems in various application domains.
 - Symbolic summation and sequences, geometry and discrete mathematics, programs and computational systems, ...
- Theoretical frameworks and practical tools.
 - Computer algebra and automated reasoning software.

Prerequisites for the algorithmization and automation of mathematics.

Contents

What are you going to see?

- Symbolic Summation and the Modeling of Sequences.
 - Carsten Schneider.
- Logic Models of Problems and Computations.
 - Wolfgang Schreiner.
- Modeling Problems in Geometry and Discrete Mathematics.
 - Wolfgang Windsteiger.

A (non-exhaustive) selection of topics pursued at the RISC institute.

1. Introduction

2. Symbolic Summation and the Modeling of Sequences

3. Logical Models of Problems and Computations

4. Modeling Problems in Geometry and Discrete Mathematics

- Problem 1: How to get from A to B ?
- Problem 2: How to efficiently use resources?

5. Organization

Example: a challenging email

From: Doron Zeilberger
To: Robin Pemantle, Herbert Wilf
CC: Carsten Schneider

Robin and Herb,

I am willing to bet that Carsten Schneider's SIGMA package for handling sums with harmonic numbers (among others) can do it in a jiffy. I am Cc-ing this to Carsten.

Carsten: please do it, and Cc- the answer to me.
-Doron

The problem

From: Robin Pemantle [University of Pennsylvania]

To: herb wilf; doron zeilberger

Herb, Doron,

I have a sum that, when I evaluate numerically, looks suspiciously like it comes out to exactly 1.

Is there a way I can automatically decide this?

The sum may be written in many ways, but one is:

$$\sum_{k=1}^{\infty} \frac{H_{k+1} - 1}{k(k+1)} \boxed{\sum_{j=1}^{\infty} \frac{H_j}{j(j+k)}}$$

with

$$H_j := \sum_{i=1}^j \frac{1}{i} (= H_j)$$

The summation paradigms

$$\mathbf{A}(k) = \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)}$$

The summation paradigms

$$k^2 \mathbf{A}(k) - (k+1)(2k+1) \mathbf{A}(k+1) + (k+1)(k+2) \mathbf{A}(k+2) = \frac{1}{k+1}$$

Recurrence finder

$$\mathbf{A}(k) = \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)}$$

The summation paradigms

$$k^2 \mathbf{A}(k) - (k+1)(2k+1) \mathbf{A}(k+1) + (k+1)(k+2) \mathbf{A}(k+2) = \frac{1}{k+1}$$

Recurrence solver

$$\mathbf{A}(k) = \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)} \in \left\{ c_1 \frac{H_k}{k} + c_2 \frac{1}{k} + \frac{kH_k^2 - 2H_k + kH_k^{(2)}}{2k^2} \mid c_1, c_2 \in \mathbb{R} \right\}$$

The summation paradigms

$$k^2 \mathbf{A}(k) - (k+1)(2k+1)\mathbf{A}(k+1) + (k+1)(k+2)\mathbf{A}(k+2) = \frac{1}{k+1}$$

Recurrence solver

$$\mathbf{A}(k) = \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)} = 0 \frac{H_k}{k} + \zeta(2) \frac{1}{k} + \frac{kH_k^2 - 2H_k + kH_k^{(2)}}{2k^2}$$

where

$$\zeta(z) = \sum_{i=1}^{\infty} \frac{1}{i^z} \quad H_k^{(2)} = \sum_{i=1}^k \frac{1}{i^2}$$

In[1]:= << **Sigma.m**

Sigma - A summation package by Carsten Schneider © RISC-Linz

In[2]:= **mySum** = $\sum_{k=1}^a \frac{H_k}{k(k+n)}$

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Sigma - A summation package by Carsten Schneider © RISC-Linz

$$\text{In[2]:= mySum} = \sum_{k=1}^a \frac{H_k}{k(k+n)}$$

In[3]:= rec = GenerateRecurrence[mySum, n][[1]]

$$\begin{aligned} \text{Out[3]= } n^2 \text{SUM}[n] - (n+1)(2n+1) \text{SUM}[n+1] + (n+1)(n+2) \text{SUM}[n+2] == \\ \frac{(-a-1)H_a}{(a+n+1)(a+n+2)} + \frac{a}{(n+1)(a+n+1)} \end{aligned}$$

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In[4]:= rec = LimitRec[rec, SUM[n], {n}, a]

$$\text{Out[4]= } n^2 \text{SUM}[n] - (n+1)(2n+1)\text{SUM}[n+1] + (n+1)(n+2)\text{SUM}[n+2] = \frac{1}{n+1}$$

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In[5]:= recSol = SolveRecurrence[rec, SUM[n]]

$$\text{Out[5]= } \left\{ \left\{ 0, \frac{1}{n} \right\}, \left\{ 0, \frac{\sum_{i=1}^n \frac{1}{i}}{n} - \frac{1}{n^2} \right\}, \left\{ 1, \frac{\left(\sum_{i=1}^n \frac{1}{i} \right)^2}{2n} - \frac{\sum_{i=1}^n \frac{1}{i}}{n^2} + \frac{\sum_{i=1}^n \frac{1}{i^2}}{2n} \right\} \right\}$$

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In[6]:= FindLinearCombination[recSol, {1, {\zeta_2, 1/2 + \zeta_2/2}}, n, 2]

$$\text{Out[6]= } -\frac{\sum_{i=1}^n \frac{1}{i}}{n^2} + \frac{\left(\sum_{i=1}^n \frac{1}{i}\right)^2}{2n} + \frac{\sum_{i=1}^n \frac{1}{i^2}}{2n} + \frac{\zeta_2}{n}$$

Example

$$S = \sum_{k=1}^{\infty} \frac{H_{k+1} - 1}{k(k+1)} \underbrace{\left[\sum_{j=1}^{\infty} \frac{H_j}{j(j+k)} \right]}_{= \frac{\zeta(2)}{k} + \frac{kH_k^2 - 2H_k + kH_k^{(2)}}{2k^2}}$$

Example

$$\begin{aligned} S &= \sum_{k=1}^{\infty} \frac{H_{k+1} - 1}{k(k+1)} \underbrace{\left[\sum_{j=1}^{\infty} \frac{H_j}{j(j+k)} \right]} \\ &= \frac{\zeta(2)}{k} + \frac{kH_k^2 - 2H_k + kH_k^{(2)}}{2k^2} \\ &= -4\zeta(2) + (\zeta(2) - 1) \sum_{i=1}^{\infty} \frac{H_i}{i^2} - \sum_{i=1}^{\infty} \frac{H_i^2}{i^3} + \frac{1}{2} \sum_{i=1}^{\infty} \frac{H_i^3}{i^2} + \frac{1}{2} \sum_{i=1}^{\infty} \frac{H_i H_i^{(2)}}{i^2} \end{aligned}$$

Example

$$\begin{aligned} S &= \sum_{k=1}^{\infty} \frac{H_{k+1} - 1}{k(k+1)} \underbrace{\left[\sum_{j=1}^{\infty} \frac{H_j}{j(j+k)} \right]} \\ &= \frac{\zeta(2)}{k} + \frac{kH_k^2 - 2H_k + kH_k^{(2)}}{2k^2} \\ &= -4\zeta(2) + (\zeta(2) - 1) \sum_{i=1}^{\infty} \frac{H_i}{i^2} - \sum_{i=1}^{\infty} \frac{H_i^2}{i^3} + \frac{1}{2} \sum_{i=1}^{\infty} \frac{H_i^3}{i^2} + \frac{1}{2} \sum_{i=1}^{\infty} \frac{H_i H_i^{(2)}}{i^2} \\ &= -4\zeta(2) - 2\zeta(3) + 4\zeta(2)\zeta(3) + 2\zeta(5) = 0.999222\dots \end{aligned}$$

The basic idea (special case telescoping)

FIND $g(k)$:

$$H_k = g(k+1) - g(k)$$

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A difference ring for the **summand**:

Construct a formal ring

$$\mathbb{A} := \underbrace{\mathbb{Q}(x)}_{\text{rat. fu. field}} [s]$$

polynomial ring

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FIND $g(k)$:

$$H_k = g(k+1) - g(k)$$

A difference ring for the **summand**:

Construct a formal ring

$$\mathbb{A} := \mathbb{Q}(x)[s]$$

and a ring automorphism $\sigma : \mathbb{A} \rightarrow \mathbb{A}$ defined by

$$\sigma(c) = c \quad \forall c \in \mathbb{Q},$$

$$\sigma(x) = x + 1,$$

$$\sigma(s) = s + \frac{1}{x+1},$$

$$\mathcal{S} k = k + 1,$$

$$\mathcal{S} H_k = H_k + \frac{1}{k+1}.$$

The basic idea (special case telescoping)

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A difference ring for the **summand**:

Construct a formal ring

(\mathbb{A}, σ) *RPIΣ-ring*

$$\mathbb{A} := \mathbb{Q}(x)[s]$$

Karr 1981, Schneider 2001–

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$$\mathcal{S}k = k + 1,$$

$$\mathcal{S}H_k = H_k + \frac{1}{k+1}.$$

with


$$\text{const}_\sigma(\mathbb{A}) = \{c \in \mathbb{A} \mid \sigma(c) = c\} = \mathbb{Q}$$

The basic idea (special case telescoping)

GIVEN FIND $g(k)$:

$$H_k = g(k+1) - g(k)$$

FIND $g \in \mathbb{A}$:


$$s = \sigma(g) - g$$

The basic idea (special case telescoping)

GIVEN FIND $g(k)$:

$$H_k = g(k+1) - g(k)$$

FIND $g \in \mathbb{A}$:

$$s = \sigma(g) - g$$

recursive ansatz

$$g = x s - x$$

The basic idea (special case telescoping)

GIVEN FIND $g(k)$:

$$H_k = g(k+1) - g(k)$$

FIND $g \in \mathbb{A}$:

$$x \equiv k$$

$$s \equiv H_k$$

$$s = \sigma(g) - g$$

recursive ansatz

$$g = x s - x$$

The basic idea (special case telescoping)

GIVEN FIND $g(k)$:

$$H_k = g(k + 1) - g(k)$$

Summation of the telescoping equation over k from 1 to n yields

$$\sum_{k=1}^n H_k = g(n + 1) - g(1)$$

The basic idea (special case telescoping)

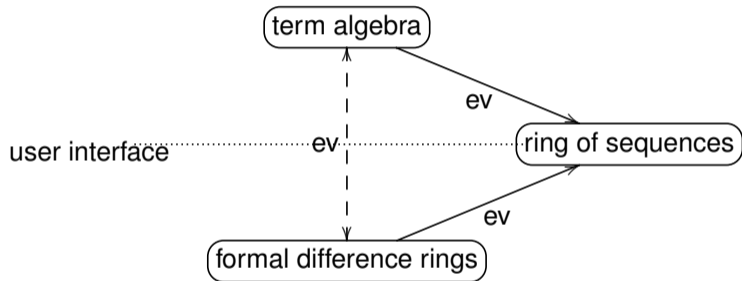
GIVEN FIND $g(k)$:

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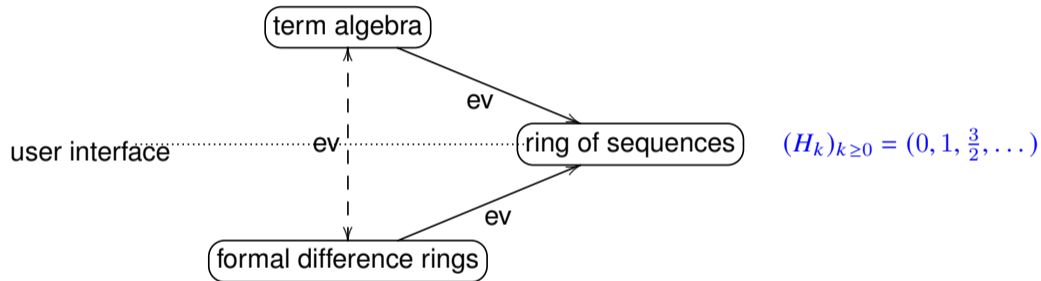
Summation of the telescoping equation over k from 1 to n yields

$$\sum_{k=1}^n H_k = g(n+1) - g(1)$$
$$= (n+1)H_{n+1} - (n+1).$$

Modeling of sequences (built by nested sums/products)

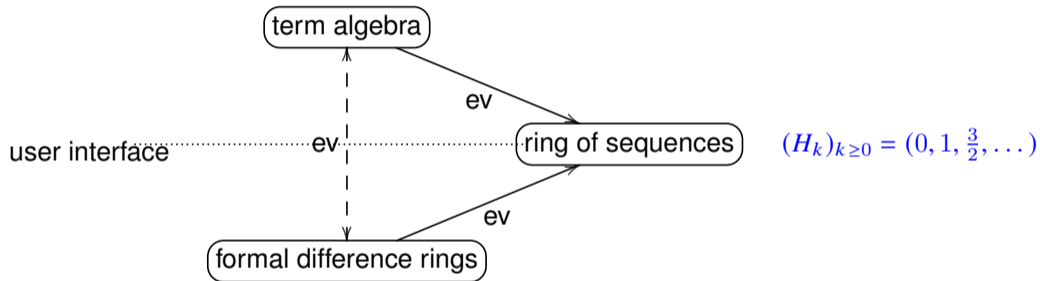


Modeling of sequences (built by nested sums/products)



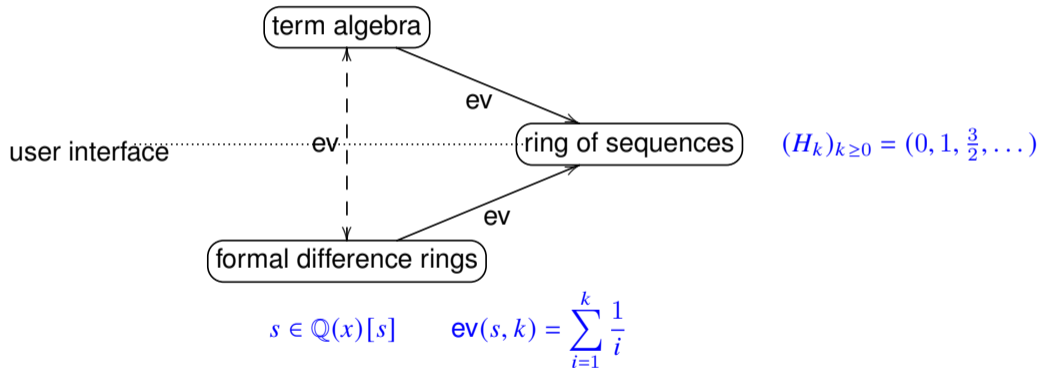
Modeling of sequences (built by nested sums/products)

$$H = \text{Sum}(1, \frac{1}{x}) \quad \text{ev}(H, k) = \sum_{i=1}^k \frac{1}{i}$$



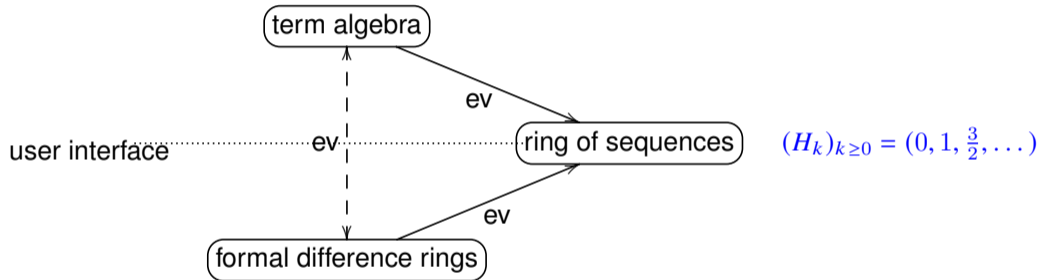
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Modeling of sequences (built by nested sums/products)

$$H = \text{Sum}(1, \frac{1}{x}) \quad \text{ev}(H, k) = \sum_{i=1}^k \frac{1}{i}$$



$$s \in \mathbb{Q}(x)[s] \quad \text{ev}(s, k) = \sum_{i=1}^k \frac{1}{i}$$

computer algebra algorithms
(for unique representations,
recurrence finding and solving)

Possible proseminar topics

1. Carry out a concrete (non-trivial example) and present details on the different modeling layers
2. Elaborate on canonical simplifiers (unique representation) and the simplification of summation objects in the difference ring setting
3. The interaction of term algebras and computer algebra
4. Elaborate on the modeling of sequences with the holonomic approach (representation of sequences by recurrences and initial values)

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In[3]:= << **EvaluateMultiSums.m**

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In[4]:= **EvaluateMultiSum** $\left[\sum_{n=1}^{\infty} \sum_{k=1}^{\infty} \frac{H_k (H_{n+1} - 1)}{kn(n+1)(k+n)} \right]$

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Out[4]= $-4\zeta_2 - 2\zeta_3 + 4\zeta_2\zeta_3 + 2\zeta_5$

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In[5]:= **EvaluateMultiSum** $\left[\sum_{n=1}^{\infty} \sum_{k=1}^{\infty} \frac{H_k^2 (H_{n+1} - 1)^2}{k(k+n)n}\right]$

Out[5]= $-10\zeta_3 + \zeta_2^2 \left(\frac{58\zeta_3}{5} - \frac{29}{5}\right) - 10\zeta_5 + \zeta_2(-\zeta_3 + 13\zeta_5 - 4) + \frac{457\zeta_7}{8}$

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In[5]:= **EvaluateMultiSum** $\left[\sum_{n=1}^{\infty} \sum_{k=1}^{\infty} \frac{H_k (H_{n+1} - 1)}{k(k+n)^2 n^2}\right]$

Out[5]= $2\zeta_3 + \zeta_2^2 \left(\frac{17\zeta_3}{10} + \frac{17}{10}\right) + \zeta_2(2\zeta_3 - 3\zeta_5 - 4) - \frac{9\zeta_5}{2} + \frac{3\zeta_7}{16}$

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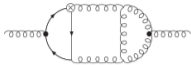
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Out[5]= $3\zeta_3^2 - \frac{15\zeta_5}{2} + \zeta_2(9\zeta_5 - 6\zeta_3) + \frac{149\zeta_7}{16} + \frac{114}{35}\zeta_2^3$

Applications:

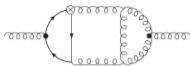
- analysis of algorithms (QuickSort, AVL trees, ...)
- combinatorial problems
- number theory
- numerics
- statistics
- special functions
- complex analysis
- \vdots
- **particle physics**

Application: Evaluation of Feynman integrals



Behavior of particles

Application: Evaluation of Feynman integrals



Behavior of particles



$$\int \Phi(N, \epsilon, x) dx$$

Feynman integrals

Feynman integrals

$$\int_0^1 x^N dx$$

Feynman integrals

$$\int_0^1 x^N (1+x)^N dx$$

Feynman integrals

$$\int_0^1 \frac{x^N (1+x)^N}{(1-x)^{1+\varepsilon}} dx$$

Feynman integrals

$$\int_0^1 \int_0^1 \frac{x_1^N (1+x_1)^N}{(1-x_1)^{1+\varepsilon}} \dots dx_1 dx_2$$

Feynman integrals

$$\int_0^1 \int_0^1 \int_0^1 \frac{x_1^N (1+x_1)^N}{(1-x_1)^{1+\varepsilon}} \dots dx_1 dx_2 dx_3$$

Feynman integrals

$$\int_0^1 \int_0^1 \int_0^1 \int_0^1 \frac{x_1^N (1+x_1)^N}{(1-x_1)^{1+\varepsilon}} \dots dx_1 dx_2 dx_3 dx_4$$

Feynman integrals

$$\int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \frac{x_1^N (1+x_1)^N}{(1-x_1)^{1+\varepsilon}} \dots dx_1 dx_2 dx_3 dx_4 dx_5$$

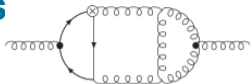
Feynman integrals

$$\int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \frac{x_1^N (1+x_1)^N}{(1-x_1)^{1+\varepsilon}} \dots dx_1 dx_2 dx_3 dx_4 dx_5 dx_6$$

Feynman integrals

$$\sum_{j=0}^{N-3} \sum_{k=0}^j \binom{N-1}{j+2} \binom{j+1}{k+1} \\ \times \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \frac{x_1^N (1+x_1)^{N-j+k}}{(1-x_1)^{1+\varepsilon}} \dots dx_1 dx_2 dx_3 dx_4 dx_5 dx_6$$

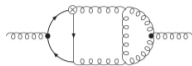
Feynman integrals



a 3-loop massive ladder diagram
[arXiv:1509.08324]

$$\begin{aligned}
 & \sum_{j=0}^{N-3} \sum_{k=0}^j \binom{N-1}{j+2} \binom{j+1}{k+1} \quad || \\
 & \times \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \theta(1-x_5-x_6)(1-x_2)(1-x_4)x_2^{-\varepsilon} \\
 & (1-x_2)^{-\varepsilon} x_4^{\varepsilon/2-1} (1-x_4)^{\varepsilon/2-1} x_5^{\varepsilon-1} x_6^{-\varepsilon p/2} \\
 & \left[\begin{aligned}
 & [-x_3(1-x_4) - x_4(1-x_5-x_6+x_5x_1+x_6x_3)]^k \\
 & + [x_3(1-x_4) - (1-x_4)(1-x_5-x_6+x_5x_1+x_6x_3)]^k
 \end{aligned} \right] \\
 & \times (1-x_5-x_6+x_5x_1+x_6x_3)^{j-k} (1-x_2)^{N-3-j}
 \end{aligned}$$

Application: Evaluation of Feynman integrals



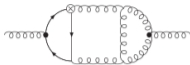
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$$\int \Phi(N, \epsilon, x) dx$$

Feynman integrals

Application: Evaluation of Feynman integrals



Behavior of particles



$$\int \Phi(N, \epsilon, x) dx$$

Feynman integrals

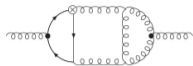


DESY

$$\sum f(N, \epsilon, k)$$

complicated
multi-sums

Application: Evaluation of Feynman integrals



Behavior of particles



$$\int \Phi(N, \epsilon, x) dx$$

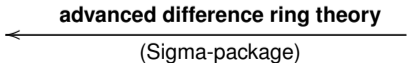
Feynman integrals



DESY

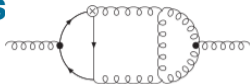
$$\sum f(N, \epsilon, k)$$

complicated
multi-sums



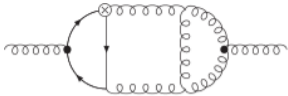
expression in
special functions

Feynman integrals

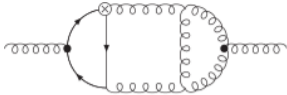


a 3-loop massive ladder diagram
[arXiv:1509.08324]

$$\begin{aligned}
 & \sum_{j=0}^{N-3} \sum_{k=0}^j \binom{N-1}{j+2} \binom{j+1}{k+1} \quad || \\
 & \times \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \theta(1-x_5-x_6)(1-x_2)(1-x_4)x_2^{-\varepsilon} \\
 & (1-x_2)^{-\varepsilon} x_4^{\varepsilon/2-1} (1-x_4)^{\varepsilon/2-1} x_5^{\varepsilon-1} x_6^{-\varepsilon p/2} \\
 & \left[\begin{aligned}
 & [-x_3(1-x_4) - x_4(1-x_5-x_6+x_5x_1+x_6x_3)]^k \\
 & + [x_3(1-x_4) - (1-x_4)(1-x_5-x_6+x_5x_1+x_6x_3)]^k
 \end{aligned} \right] \\
 & \times (1-x_5-x_6+x_5x_1+x_6x_3)^{j-k} (1-x_2)^{N-3-j}
 \end{aligned}$$



$$= F_{-3}(N)\varepsilon^{-3} + F_{-2}(N)\varepsilon^{-2} + F_{-1}(N)\varepsilon^{-1} + \boxed{F_0(N)}$$



$$= F_{-3}(N)\varepsilon^{-3} + F_{-2}(N)\varepsilon^{-2} + F_{-1}(N)\varepsilon^{-1} + \boxed{F_0(N)}$$

Simplify

||

$$\sum_{j=0}^{N-3} \sum_{k=0}^j \sum_{l=0}^k \sum_{q=0}^{-j+N-3} \sum_{s=1}^{-l+N-q-3} \sum_{r=0}^{-l+N-q-s-3} (-1)^{-j+k-l+N-q-3} \times$$

$$\times \frac{\binom{j+1}{k+1} \binom{k}{l} \binom{N-1}{j+2} \binom{-j+N-3}{q} \binom{-l+N-q-3}{s} \binom{-l+N-q-s-3}{r} r! (-l+N-q-r-s-3)! (s-1)!}{(-l+N-q-2)! (-j+N-1) (N-q-r-s-2) (q+s+1)}$$

$$\left[4H_{-j+N-1} - 4H_{-j+N-2} - 2H_k - (H_{-l+N-q-2} + H_{-l+N-q-r-s-3} - 2H_{r+s}) \right.$$

$$\left. + 2H_{s-1} - 2H_{r+s} \right] + \mathbf{3 \text{ further 6-fold sums}}$$

$$\boxed{F_0(N)} =$$

$$\begin{aligned}
& \frac{7}{12} S_1(N)^4 + \frac{(17N+5)S_1(N)^3}{3N(N+1)} + \left(\frac{35N^2-2N-5}{2N^2(N+1)^2} + \frac{13S_2(N)}{2} + \frac{5(-1)^N}{2N^2} \right) S_1(N)^2 \\
& + \left(-\frac{4(13N+5)}{N^2(N+1)^2} + \left(\frac{4(-1)^N(2N+1)}{N(N+1)} - \frac{13}{N} \right) S_2(N) + \left(\frac{29}{3} - (-1)^N \right) S_3(N) \right. \\
& + (2+2(-1)^N) S_{2,1}(N) - 28S_{-2,1}(N) + \frac{20(-1)^N}{N^2(N+1)} S_1(N) + \left(\frac{3}{4} + (-1)^N \right) S_2(N)^2 \\
& - 2(-1)^N S_{-2}(N)^2 + S_{-3}(N) \left(\frac{2(3N-5)}{N(N+1)} + (26+4(-1)^N) S_1(N) + \frac{4(-1)^N}{N+1} \right) \\
& + \left(\frac{(-1)^N(5-3N)}{2N^2(N+1)} - \frac{5}{2N^2} \right) S_2(N) + S_{-2}(N) (10S_1(N)^2 + \left(\frac{8(-1)^N(2N+1)}{N(N+1)} \right. \\
& + \frac{4(3N-1)}{N(N+1)} S_1(N) + \frac{8(-1)^N(3N+1)}{N(N+1)^2} + (-22+6(-1)^N) S_2(N) - \frac{16}{N(N+1)} \left. \right) \\
& + \left(\frac{(-1)^N(9N+5)}{N(N+1)} - \frac{29}{3N} \right) S_3(N) + \left(\frac{19}{2} - 2(-1)^N \right) S_4(N) + (-6+5(-1)^N) S_{-4}(N) \\
& + \left(-\frac{2(-1)^N(9N+5)}{N(N+1)} - \frac{2}{N} \right) S_{2,1}(N) + (20+2(-1)^N) S_{2,-2}(N) + (-17+13(-1)^N) S_{3,1}(N) \\
& - \frac{8(-1)^N(2N+1)+4(9N+1)}{N(N+1)} S_{-2,1}(N) - (24+4(-1)^N) S_{-3,1}(N) + (3-5(-1)^N) S_{2,1,1}(N) \\
& + 32S_{-2,1,1}(N) + \left(\frac{3}{2} S_1(N)^2 - \frac{3S_1(N)}{N} + \frac{3}{2} (-1)^N S_{-2}(N) \right) \zeta(2)
\end{aligned}$$

$$F_0(N) =$$

$$\begin{aligned}
& \frac{7}{12} S_1(N)^4 + \frac{(17N+5)S_1(N)^3}{3N(N+1)} + \left(\frac{35N^2-2N-5}{2N^2(N+1)^2} + \frac{13S_2(N)}{2} + \frac{5(-1)^N}{2N^2} \right) S_1(N)^2 \\
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& + \left(\frac{(-1)^N(5-3N)}{2N^2(N+1)} - \frac{5}{2N^2} \right) S_2(N) + S_{-2}(N) (10S_1(N)^2 + \left(\frac{8(-1)^N(2N+1)}{N(N+1)} \right. \\
& + \frac{4(3N-1)}{N(N+1)} \left. \right) S_1(N) + \frac{8(-1)^N(3N+1)}{N(N+1)^2} + \left(-22+6(-1)^N \right) S_2(N) - \frac{16}{N(N+1)} \\
& + \left(\frac{(-1)^N(9N+5)}{N(N+1)} - \frac{29}{3N} \right) S_3(N) + \left(\frac{19}{2} - 2(-1)^N \right) S_4(N) + \left(-6+5(-1)^N \right) S_{-4}(N) \\
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\end{aligned}$$

$$F_0(N) =$$

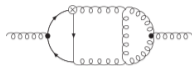
$$\begin{aligned}
 & \frac{7}{12} S_1(N)^4 + \frac{(17N+5)S_1(N)^3}{3N(N+1)} + \left(\frac{35N^2-2N-5}{2N^2(N+1)^2} + \frac{13S_2(N)}{2} + \frac{5(-1)^N}{2N^2} \right) S_1(N)^2 \\
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 & \left. - 2(-1)^N S_{-2}(N)^2 + S_{-3}(N) \left(\frac{2(3N-5)}{N(N+1)} + (20+4(-1)^N) S_1(N) \right) \right) S_2(N) = \sum_{i=1}^N \frac{1}{i^2} \\
 & + \left(\frac{(-1)^N(5-3N)}{2N^2(N+1)} - \frac{5}{2N^2} \right) S_2(N) + S_{-2}(N) (10S_1(N)^2 + \frac{8(-1)^N}{N(N+1)} \\
 & + \frac{4(3N-1)}{N(N+1)}) S_1(N) + \frac{8(-1)^N(3N+1)}{N(N+1)^2} + (-22+6(-1)^N) S_2(N) - \frac{16}{N(N+1)} \\
 & + \left(\frac{(-1)^N(9N+5)}{N(N+1)} - \frac{29}{3N} \right) S_3(N) + \left(\frac{19}{2} - 2(-1)^N \right) S_4(N) + (-6+5(-1)^N) S_{-4}(N) \\
 & + \left(-\frac{2(-1)^N(9N+5)}{N(N+1)} - \frac{2}{N} \right) S_{2,1}(N) + (20+2(-1)^N) S_{2,-2}(N) + (-17+13(-1)^N) S_{3,1}(N) \\
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 & + \left(\frac{(-1)^N(5-3N)}{2N^2(N+1)} - \frac{5}{2N^2} \right) S_2(N) + S_{-2}(N) (10S_1(N)^2 + \left(\frac{8(-1)^N}{N(N+1)} \right. \\
 & \left. + \frac{4(3N-1)}{N(N+1)} \right) S_1(N) + \frac{8(-1)^N(3N-1)}{N(N+1)} S_1(N) \\
 & + \left(\frac{(-1)^N(9N+5)}{N(N+1)} - \frac{29}{3N} \right) S_3(N) + \left(\frac{(-1)^N(9N+5)}{N(N+1)} - \frac{2}{N} \right) S_{2,1}(N) \\
 & + \left(\frac{2(-1)^N(9N+5)}{N(N+1)} - \frac{2}{N} \right) S_{2,1}(N) - \frac{8(-1)^N(2N+1)+4(9N+1)}{N(N+1)} S_{-2,1,1}(N) \\
 & + 32S_{-2,1,1}(N) + \left(\frac{3}{2} S_1(N)^2 - \frac{3S_1(N)}{N} + \frac{3}{2} (-1)^N S_{-2}(N) \right) \zeta(2)
 \end{aligned}$$

$S_1(N) = \sum_{i=1}^N \frac{1}{i}$
 $S_2(N) = \sum_{i=1}^N \frac{1}{i^2}$
 $S_{-2,1,1}(N) = \sum_{i=1}^N \frac{(-1)^i \sum_{j=1}^i \sum_{k=1}^j \frac{1}{k}}{i^2}$

Application: Evaluation of Feynman integrals



Behavior of particles



$$\int \Phi(N, \epsilon, x) dx$$

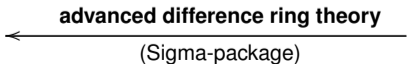
Feynman integrals



DESY

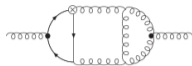
$$\sum f(N, \epsilon, k)$$

complicated
multi-sums



expression in
special functions

Application: Evaluation of Feynman integrals



Behavior of particles



$$\int \Phi(N, \epsilon, x) dx$$

Feynman integrals



LHC at CERN



DESY

$$\sum f(N, \epsilon, k)$$

complicated
multi-sums

applicable

expression in
special functions

advanced difference ring theory

(Sigma-package)

1. Introduction

2. Symbolic Summation and the Modeling of Sequences

3. Logical Models of Problems and Computations

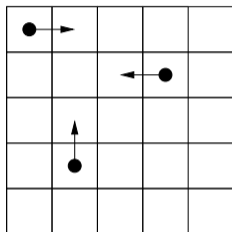
4. Modeling Problems in Geometry and Discrete Mathematics

- Problem 1: How to get from A to B ?
- Problem 2: How to efficiently use resources?

5. Organization

Example: A Robotic System

An grid in which multiple robots move around.



- **System:** each robot moves one cell in a selected direction.
- **Safety:** the robots shall not collide with the walls or with each other.

Our task is to model an adequate control software for each robot: given the current situation of the system, compute a safe direction for the movement of the robot.

A Model of the System

A hybrid logical/operational system description.

```
shared system Robots
{
  var x: Positions; var y: Positions;
  invariant noCollision(x, y);

  init(x0:Positions, y0:Positions) with initialState(x0, y0);
  {
    x := x0; y := y0;
  }

  action move(r:Robot, d:Direction) with nextDir(x, y, r, d);
  {
    x := moveX(x, r, d); y := moveY(y, r, d);
  }
}
```

Control software is specified (implicitly defined) by predicate `nextDir()`.

Auxiliary Definitions

```
val R: N; // number of robots
val P: N; // number of positions
axiom notzero  $\Leftrightarrow R \geq 1 \wedge P \geq 1$ ;

type Robot = N[R-1];
type Position = N[P-1];
type Positions = Array[R,Position];
type Direction = N[4];
val Stop = 0; val Left = 1; val Right = 2; val Up = 3; val Down = 4;

pred noCollision(x:Positions, y:Positions)  $\Leftrightarrow$ 
   $\forall r1:Robot, r2:Robot \text{ with } r1 < r2. x[r1] \neq x[r2] \vee y[r1] \neq y[r2]$ ;

fun moveX(x:Positions, r:Robot, d: Direction): Positions =
  if d = Left then x with [r] = x[r]-1 else
  if d = Right then x with [r] = x[r]+1 else x;
fun moveY(y:Positions, r:Robot, d: Direction):Positions =
  if d = Up then y with [r] = y[r]-1 else
  if d = Down then y with [r] = y[r]+1 else y;
```

The Control Software

```
// an initial state of the system
pred initialState(x: Positions, y:Positions)  $\Leftrightarrow$  noCollision(x, y);

// any robot different from r may move to position xr, yr
pred anyOtherAt(x:Positions, y:Positions, r:Robot, xr:Position, yr:Position)  $\Leftrightarrow$ 
   $\exists r0$ : Robot with  $r0 \neq r$ .  $xr = x[r0] \wedge yr = y[r0]$ ;

// the relation between the current system state and the new direction d of robot r
pred nextDir(x:Positions, y:Positions, r:Robot, d:Direction)  $\Leftrightarrow$ 
  (d = Left  $\Rightarrow x[r] > 0 \wedge \neg$ anyOtherAt(x, y, r, x[r]-1, y[r]))
 $\wedge$  (d = Right  $\Rightarrow x[r] < P-1 \wedge \neg$ anyOtherAt(x, y, r, x[r]+1, y[r]))
 $\wedge$  (d = Up  $\Rightarrow y[r] > 0 \wedge \neg$ anyOtherAt(x, y, r, x[r], y[r]-1))
 $\wedge$  (d = Down  $\Rightarrow y[r] < P-1 \wedge \neg$ anyOtherAt(x, y, r, x[r], y[r]+1));
```

The robot may move within the grid to any unoccupied position.

Verifying the Safety of the System

Using R=3.

Using P=5.

Executing system Robots.

13699 system states visited...

13800 system states found with search depth 13062.

Execution completed (3170 ms).

Checking the safety of all reachable states of the systems.

Verification Conditions

Alternative: checking the validity of verification conditions.

```
theorem _Robots_6_initPre_cverify_0(x:Positions, y:Positions)
  ⇔ ∀x0:Map[ℤ[0,2],ℤ[0,4]], y0:Map[ℤ[0,2],ℤ[0,4]].
    (initialState(x0,y0) ⇒ (let x = x0 in (let y = y0 in noCollision(x,y)))));
```

```
theorem _Robots_6_actionPre_0_cverify_0(x:Positions, y:Positions)
  requires noCollision(x, y);
  ⇔ ∀r:ℤ[0,2], d:ℤ[0,4]. (nextDir(x,y,r,d) ⇒
    (let x = moveX(x,r,d) in (let y = moveY(y,r,d) in noCollision(x,y)))));
```

The SMT solver Yices started execution.

Theorem is valid (5 ms, translation: 1 ms, decision: 2 ms).

The SMT solver Yices started execution.

Theorem is valid (36 ms, translation: 5 ms, decision: 27 ms).

By formally *proving* such conditions, we can also verify *infinite* state systems.

A Purely Logical Model of the System

```
pred nextState(x:Positions, y:Positions, x0:Positions, y0:Positions)  $\Leftrightarrow$   
   $\exists r$ :Robot, d:Direction with nextDir(x, y, r, d).  
    x0 = moveX(x, r, d)  $\wedge$  y0 = moveY(y, r, d);
```

```
shared system RobotsLogical  
{  
  var x: Positions; var y: Positions;  
  invariant noCollision(x, y);  
  init()  $\Leftrightarrow$  initialState(x0, y0);  
  action move()  $\Leftrightarrow$  nextState(x, y, x0, y0);  
}
```

```
theorem _RobotsLogical_8_initPre_pverify_0(x:Positions, y:Positions)  
 $\Leftrightarrow \forall x0$ :Map[Z[0,2],Z[0,4]],  $y0$ :Map[Z[0,2],Z[0,4]]. (initialState(x0, y0)  $\Rightarrow$   
  (letpar x = x0, y = y0 in noCollision(x, y)));
```

```
theorem _RobotsLogical_8_actionPre_0_pverify_0(x:Positions, y:Positions)  
  requires noCollision(x, y);
```

```
 $\Leftrightarrow \forall x0$ :Map[Z[0,2],Z[0,4]],  $y0$ :Map[Z[0,2],Z[0,4]].
```

```
  (nextState(x, y, x0, y0)  $\Rightarrow$  (letpar x = x0, y = y0 in noCollision(x, y)));
```


Course Contents

Formulating logical formulas that characterize computational problems/systems.

- Logical specification of computational problems.

- Pre- and post-conditions.
- Validation of specifications according to various criteria.
- Computation of results by evaluation of logical formulas.

- Logical modeling of computational systems.

- Initial state conditions, transition relations.
- Modeling safety properties respectively goal states.
- Computation of results by state space traversal.

Software: the “mathematical model checker” RISCAL.

RISCAL: RISC Algorithm Language

The screenshot displays the RISCAL Algorithm Language (RISCAL) interface. The main window is titled "RISC Algorithm Language (RISCAL)".

File: /usr2/schreine/papers/RISCALBook/src/.../models/gcd.txt

Code Editor: Contains RISCAL source code for a GCD function. It includes comments like "Euclid's algorithm as a recursive function" and "simplified version". The code defines a recursive function `gcdf` and a procedure `gcdp`.

Analysis Panel: Shows configuration options for the analysis process.

- Translation: Nondeterminism Default Value: 0 Other Values: [...]
- Execution: Silent Inputs: Per Millie: Branches: Depth:
- Visualization: Trace Tree Width: 400 Height: 400
- Parallelism: Multi-Threaded Threads: 4 Distributed Servers: [...]
- Operation: `gcdp(Z,Z)`

Output Panel: Displays the execution results for the operation `gcdp(Z,Z)`.

RISC ALGORITHM LANGUAGE 3.1 (APRIL 20, 2020)
<http://www.risc.jku.at/research/formal/software/RISCAL>
(C) 2016 - Research Institute for Symbolic Computation (RISC)
This is free software distributed under the terms of the GNU GPL.
Execute "RISCAL -h" to see the available command line options.

Reading file /usr2/schreine/papers/RISCALBook/src/.../models/gcd.txt
Using N=10.
Computing the truth value of notZero...
Computing the value of zero...
Computing the truth value of twoNums...
Computing the truth value of zeroMin...
Type checking and translation completed.
Executing gcdp 27 Spec(Z,Z) with all 121 inputs.
Execution completed for ALL inputs (148 ms, 120 checked, 1 inadmissible).
Executing gcdp 27 PreSat().
Execution completed (1 ms).
Executing gcdp 27 PreNotTrivial().
Execution completed (0 ms).
Executing gcdp 27 PostSat(Z,Z) with all 121 inputs.
Execution completed for ALL inputs (112 ms, 120 checked, 1 inadmissible).
Executing gcdp 27 PostNotTrivialAll(Z,Z) with all 121 inputs.
Execution completed for ALL inputs (68 ms, 120 checked, 1 inadmissible).
Executing gcdp 27 PostNotTrivialSome().
Execution completed (0 ms).
Executing gcdp 27 PostUnique(Z,Z) with all 121 inputs.
Execution completed for ALL inputs (355 ms, 120 checked, 1 inadmissible).

Tasks Panel: Lists tasks for the operation `gcdp(Z,Z)`.

- Execute operation
- Validate specification
 - Execute specification
 - Is precondition satisfiable?
 - Is precondition not trivial?
 - Is postcondition always satisfiable?
 - Is postcondition always not trivial?
 - Is postcondition sometimes not trivial?
 - Is result uniquely determined?
 - Verify specification preconditions
 - Verify correctness of result
 - Is result correct?
 - Verify iteration and recursion
 - Does loop invariant initially hold?
 - Does loop invariant initially hold?
 - Is loop measure non-negative?
 - Is loop invariant preserved?
 - Is loop invariant preserved?
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 - Is loop measure decreased?
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 - Verify implementation preconditions
 - Does operation precondition hold?
 - Does operation precondition hold?

A language and checker for mathematical models and algorithms.

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MODELING PROBLEMS IN GEOMETRY AND DISCRETE MATHEMATICS



PROBLEM 1: HOW TO GET FROM A TO B ?

Navigation Systems (trivial approach)

What is the mathematics behind navigation systems in modern cars?

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Solution: if no further restrictions are given, the solution is trivial: the shortest connection from A to B is the straight line from A to B , the “shortest route” is given by (A, B) with length

$$d_{\min} = \|B - A\|$$

with some appropriate norm $\|\cdot\|$.

Navigation Systems (realistic approach)

Given: start address A , destination address B , “network” of streets S .

Find: “shortest route” from A to B on S .



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Mathematical model: Given n Streets S_i with $i = 1, \dots, n$. Streets S_i and S_j intersect at crossing C_{ij} . Two crossings c and d are adjacent iff $c \neq d$ and there is no crossing between them on the same street. Two adjacent crossings are connected by a street segment.

Network of streets is characterized by

- crossings $V = \{C_{ij} \mid i, j = 1, \dots, n\}$,
- adjacency relation between crossings $E = \{\{v_1, v_2\} \mid v_1 \text{ and } v_2 \text{ are adjacent}\}$,
- length of street segments $w: E \rightarrow \mathbb{R}^+$.

Undirected Weighted Graphs

The triple $G = (V, E, w)$ is called an undirected weighted graph iff

- V is some non-empty finite set,
- $E \subset P(V)$ with $|e| = 2$ for all $e \in E$, and
- $w: E \rightarrow \mathbb{R}$.

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Our problem now becomes

Given: an undirected weighted graph $G = (V, E, w)$, $A, B \in V$.

Find: a sequence P of some length n in V such that

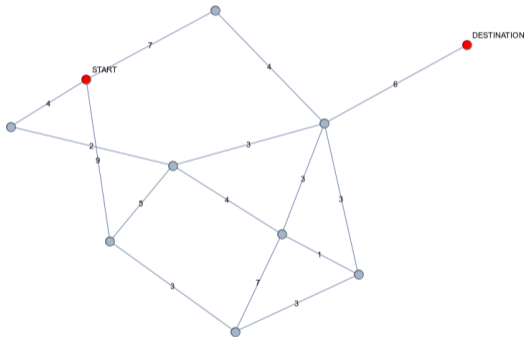
$$P_1 = A, P_n = B$$

$$\forall 1 \leq i \leq n - 1 : \{P_i, P_{i+1}\} \in E$$

$$\sum_{i=1}^n w(\{P_i, P_{i+1}\}) = \min\{w(Q) \mid Q \text{ is a path from } A \text{ to } B \text{ in } G\}$$

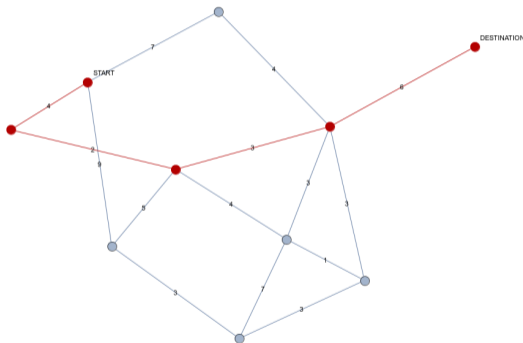
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There are several algorithms to solve the Shortest Path Problem, e.g. Dijkstra's Algorithm or the Bellman-Ford-Algorithm.

MODELING PROBLEMS IN GEOMETRY AND DISCRETE MATHEMATICS



PROBLEM 2: HOW TO EFFICIENTLY USE RESOURCES?

A Planning Problem

Real Life Situation

A factory has 10 production stations with equal capabilities. Each machine can be operated for at most 9 hours per day, production may start at 8:30. Every station needs two workers for operation, if a station stays closed the two employees can be used for other useful tasks. There are 160 orders with different production duration that have to be processed on a certain day. Each order can be processed on any of the stations. The delivery of the final products is scheduled on the night train leaving the factory no earlier than 18:00. Time for packing the products on the train is less than half an hour.

Design a “good” production schedule for that day.

Problem Analysis

- Every station can be utilized for the whole 9 hours from 8:30–17:30.

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- Every order has to be processed.
- There is no need to finish production as early as possible, finishing by 17:30 is all that is required so that the train is readily packed by 18:00.
- Fast production is not the criterion for a “good” production schedule, but the number of open production stations.

Mathematical Model

Given: orders $O = \{1, \dots, n\}$, duration $d: O \rightarrow \mathbb{R}$, stations $S = \{1, \dots, m\}$, maximal operation time on stations $D: S \rightarrow \mathbb{R}$.

Find: number of open stations k and assignment of orders to stations $s: O \rightarrow \{1, \dots, k\}$ such that

$$k \leq m, \quad (1)$$

$$\forall j \in S: \sum_{\substack{i \in O \\ s(i)=j}} d(i) \leq D(j), \quad (2)$$

$$\forall l < k \nexists t: O \rightarrow \{1, \dots, l\} \forall j \in S: \sum_{\substack{i \in O \\ t(i)=j}} d(i) \leq D(j) \quad (3)$$

(2) means assignment obeys limit on every station.

(3) means that no assignment with less stations is possible.

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There are several algorithms to solve the Bin Packing Problem, e.g. Branch-and-Bound or various Heuristic Approximation Methods, because finding the minimal k can be very time consuming.

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Organization

■ This course (VO)

- Grading based on three home assignments (3×100 grade points).
- Each assignment deals with the elaboration of a small model.
- Minimum requirement to pass the course: 3×50 grade points.
- Extra assignments: if the minimum requirements are not met.

■ Accompanying proseminar (PS)

- Deals with the kind of models treated in this course.
- Additionally discusses the basics of “mathematical practice”.
- Each participant selects an individual problem to be modeled/analyzed.
- Requirement is to write a small paper and prepare/give a small presentation.
- Some topics are also suitable for a **bachelor thesis**.

This course and the proseminar are not formally linked: they can be independently pursued and are independently graded.

Moodle Course

Central point of electronic interaction.

- Forum “Discussions”: your questions and answers.
 - Anyone can post a question or an answer.
- Forum “Announcements”: our messages.
 - Only we (the lecturers) can post here.
- Various “Assignments”: your submissions.
 - Email submissions are not accepted.
- Personal messages/emails: only for confidential matters.
 - Everything else all lecturers and students should see.

See the link in the KUSSS page of this course.