FORMAL MODELING

Algebra and Logic in Mathematical Modeling

Carsten Schneider Wolfgang Schreiner Wolfgang Windsteiger
Research Institute for Symbolic Computation (RISC)
Johannes Kepler University, Linz, Austria
FirstName.LastName@risc.jku.at

JOHANNES KEPLER
UNIVERSITY LINZ

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

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

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

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

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

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

where

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

In[1]:= << Sigma.m

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

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

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

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

Out[3]= $n^2\,\mathrm{SUM}[n] - (n+1)(2n+1)\,\mathrm{SUM}[n+1] + (n+1)(n+2)\,\mathrm{SUM}[n+2] == \frac{(-a-1)H_a}{(a+n+1)(a+n+2)} + \frac{a}{(n+1)(a+n+1)}$

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

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

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

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, {ζ_2, 1/2 + ζ_2/2}}, n, 2]**

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

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

$$= \frac{\zeta(2)}{k} + \frac{kH_k^2 - 2H_k + kH_k^{(2)}}{2k^2}$$

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$$= \frac{\zeta(2)}{k} + \frac{kH_k^2 - 2H_k + kH_k^{(2)}}{2k^2}$$

$$= -4\zeta(2) + (\zeta(2) - 1)\sum_{i=1}^{\infty} \frac{H_i}{i^2} - \sum_{i=1}^{\infty} \frac{H_i^2}{i^3} + \frac{1}{2}\sum_{i=1}^{\infty} \frac{H_i^3}{i^2} + \frac{1}{2}\sum_{i=1}^{\infty} \frac{H_i H_i^{(2)}}{i^2}$$

Example

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

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$$=-4\zeta(2)+(\zeta(2)-1)\sum_{i=1}^{\infty}\frac{H_i}{i^2}-\sum_{i=1}^{\infty}\frac{H_i^2}{i^3}+\frac{1}{2}\sum_{i=1}^{\infty}\frac{H_i^3}{i^2}+\frac{1}{2}\sum_{i=1}^{\infty}\frac{H_iH_i^{(2)}}{i^2}$$

$$=-4\zeta(2)-2\zeta(3)+4\zeta(2)\zeta(3)+2\zeta(5)=0.999222\ldots$$

The basic idea (special case telescoping)

FIND $g(k)$:

$$\boxed{H_k = g(k+1) - g(k)}$$

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A difference ring for the **summand:**

Construct a formal ring

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

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A difference ring for the **summand:**

Construct a formal ring

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

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

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

$$\sigma(x) = x + 1, \qquad \mathcal{S}\, k = k + 1,$$

$$\sigma(s) = s + \frac{1}{x+1}, \qquad \mathcal{S}\, H_k = H_k + \frac{1}{k+1}.$$

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A difference ring for the **summand:**

Construct a formal ring

$\boxed{(\mathbb{A}, \sigma)\ R\Pi\Sigma\text{-ring}}$

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Karr 1981, Schneider 2001–

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with

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

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

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recursive ansatz

$$g = x\,s - x$$

The basic idea (special case telescoping)

GIVEN FIND $g(k)$:

$$\boxed{H_k = g(k+1) - g(k)}$$

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

$x \equiv k$

$s \equiv H_k$

$$\boxed{s = \sigma(g) - g}$$

recursive ansatz

$$g = x\,s - x$$

The basic idea (special case telescoping)

GIVEN FIND $g(k)$:

$$\boxed{H_k = g(k+1) - g(k)}$$

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

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

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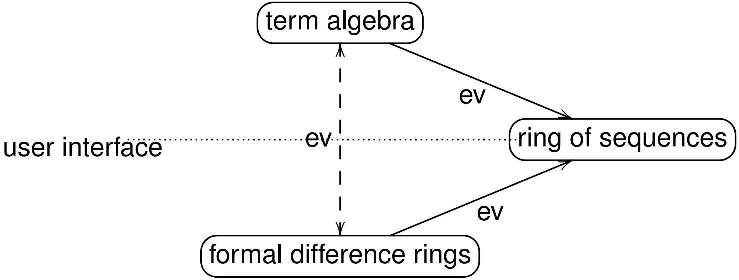
$$= (n+1)\, H_{n+1} - (n+1).$$

Modeling of sequences (built by nested sums/products)



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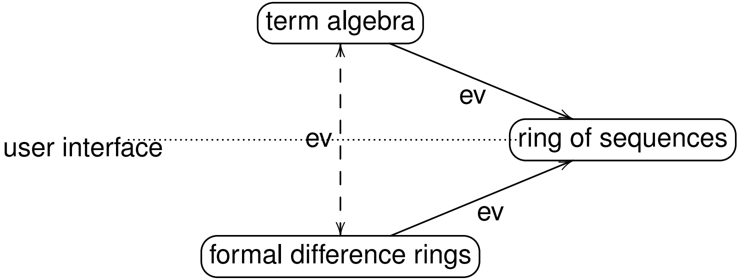
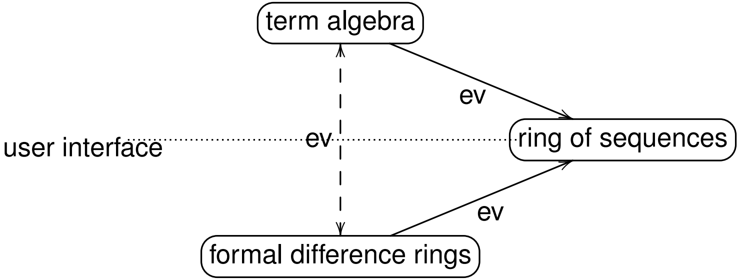


$(H_k)_{k\geq 0} = (0, 1, \frac{3}{2}, \dots)$

Modeling of sequences (built by nested sums/products)

$$H = \mathsf{Sum}(1, \tfrac{1}{x}) \qquad \mathsf{ev}(H, k) = \sum_{i=1}^{k} \frac{1}{i}$$



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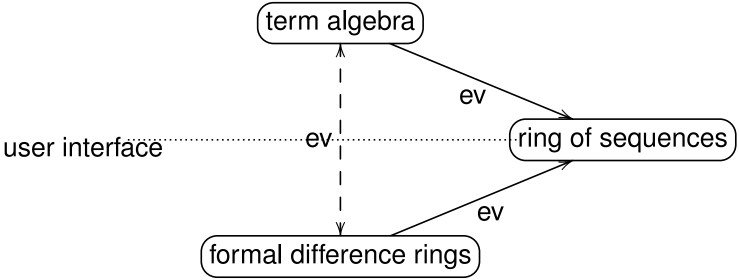

$(H_k)_{k\geq 0} = (0, 1, \frac{3}{2}, \dots)$

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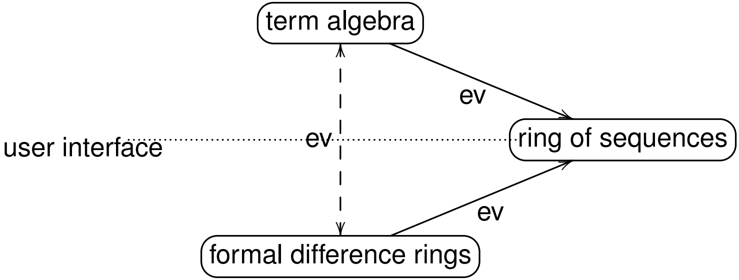

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computer algebra algorithms
(for unique representations,
recurrence finding and solving)

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)

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

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In[2]:= $<<$ **HarmonicSums.m**

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

EvaluateMultiSums by Carsten Schneider © RISC-Linz

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

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

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

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

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

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

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

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

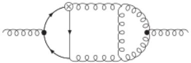
Applications:

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

  $\vdots$

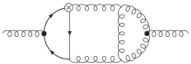
- **particle physics**

Application: Evaluation of Feynman integrals



Behavior of particles

Application: Evaluation of Feynman integrals



Behavior of particles

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

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

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

Feynman integrals

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Feynman integrals

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

Feynman integrals

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

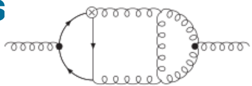
Feynman integrals

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

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]

$$\sum_{j=0}^{N-3}\sum_{k=0}^{j}\binom{N-1}{j+2}\binom{j+1}{k+1} \qquad ||$$

$$\times \int_0^1\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1 \theta(1-x_5-x_6)(1-x_2)(1-x_4)x_2^{-\varepsilon}$$

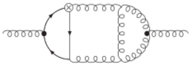
$$(1-x_2)^{-\varepsilon}x_4^{\varepsilon/2-1}(1-x_4)^{\varepsilon/2-1}x_5^{\varepsilon-1}x_6^{-ep/2}$$

$$\Big[[-x_3(1-x_4)-x_4(1-x_5-x_6+x_5x_1+x_6x_3)]^k$$

$$+[x_3(1-x_4)-(1-x_4)(1-x_5-x_6+x_5x_1+x_6x_3)]^k\Big]$$

$$\times(1-x_5-x_6+x_5x_1+x_6x_3)^{j-k}(1-x_2)^{N-3-j}$$

Application: Evaluation of Feynman integrals

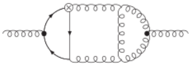


Behavior of particles

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

Feynman integrals

Application: Evaluation of Feynman integrals



Behavior of particles

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

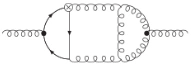
Feynman integrals

DESY

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

complicated
multi-sums

Application: Evaluation of Feynman integrals



Behavior of particles $\longrightarrow$ $\int \Phi(N,\epsilon,x)dx$

Feynman integrals

DESY $\downarrow$

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

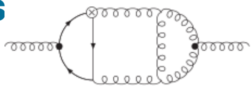
complicated multi-sums

advanced difference ring theory

(Sigma-package)

$\longleftarrow$ expression in special functions

Feynman integrals



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

$$\sum_{j=0}^{N-3}\sum_{k=0}^{j}\binom{N-1}{j+2}\binom{j+1}{k+1} \qquad \Vert$$

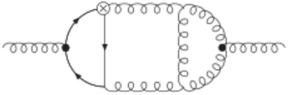
$$\times\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1 \theta(1-x_5-x_6)(1-x_2)(1-x_4)x_2^{-\varepsilon}$$

$$(1-x_2)^{-\varepsilon}x_4^{\varepsilon/2-1}(1-x_4)^{\varepsilon/2-1}x_5^{\varepsilon-1}x_6^{-ep/2}$$

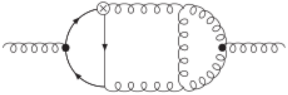
$$\Bigg[[-x_3(1-x_4)-x_4(1-x_5-x_6+x_5x_1+x_6x_3)]^k$$

$$+[x_3(1-x_4)-(1-x_4)(1-x_5-x_6+x_5x_1+x_6x_3)]^k\Bigg]$$

$$\times(1-x_5-x_6+x_5x_1+x_6x_3)^{j-k}(1-x_2)^{N-3-j}$$



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



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

Simplify $\qquad\qquad\qquad\qquad ||$

$$\boxed{\begin{aligned}&\sum_{j=0}^{N-3}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{q=0}^{-j+N-3}\sum_{s=1}^{-l+N-q-3}\sum_{r=0}^{-l+N-q-s-3}(-1)^{-j+k-l+N-q-3}\times\\ &\times\frac{\binom{j+1}{k+1}\binom{k}{l}\binom{N-1}{j+2}\binom{-j+N-3}{q}\binom{-l+N-q-3}{s}\binom{-l+N-q-s-3}{r}r!(-l+N-q-r-s-3)!(s-1)!}{(-l+N-q-2)!(-j+N-1)(N-q-r-s-2)(q+s+1)}\\ &\Bigg[4H_{-j+N-1}-4H_{-j+N-2}-2H_k-(H_{-l+N-q-2}+H_{-l+N-q-r-s-3}-2H_{r+s})\\ &+2H_{s-1}-2H_{r+s}\Bigg]+\textbf{3 further 6–fold sums}\end{aligned}}$$

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

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

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

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

$$S_1(N) = \sum_{i=1}^{N} \frac{1}{i}$$

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

$$\frac{7}{12}S_1(N)^4 + \frac{(17N+5)S_1(N)^3}{3N(N+1)} + \Big(\frac{35N^2-2N-5}{2N^2(N+1)^2} + \frac{13S_2(N)}{2} + \frac{5(-1)^N}{2N^2}\Big)S_1(N)^2$$

$$+ \Big(-\frac{4(13N \ldots}{N^2(N \ldots} \ldots \frac{\ldots N+1)}{\ldots 1)} - \frac{13}{N}\Big)S_2(N) + \Big(\frac{29}{3} - (-1)^N\Big)S_3(N)$$

$$+ \big(2+2(-1)^{\ldots} \ldots (N) + \frac{20(-1)^N}{N^2(N+1)}\Big)S_1(N) + \Big(\frac{3}{\ldots} \ldots (-1)^N\big)S_{\ldots}(N)^2$$

$$- 2(-1)^N S_{-2}(N)^2 + S_{-3}(N)\Big(\frac{2(3N-5)}{N(N+1)} + \big(26+4(-1)^N\big)S_1(N \ldots$$

$$+ \Big(\frac{(-1)^N(5-3N)}{2N^2(N+1)} - \frac{5}{2N^2}\Big)S_2(N) + S_{-2}(N)\Big(10S_1(N)^2 + \Big(\frac{8(-1 \ldots}{N(N+1)}$$

$$+ \frac{4(3N-1)}{N(N+1)}\Big)S_1(N) + \frac{8(-1)^N(3N+1)}{N(N+1)^2} + \big(-22+6(-1)^N\big)S_2(N) - \frac{16}{N(N+1)}\Big)$$

$$+ \Big(\frac{(-1)^N(9N+5)}{N(N+1)} - \frac{29}{3N}\Big)S_3(N) + \Big(\frac{19}{2} - 2(-1)^N\Big)S_4(N) + \big(-6+5(-1)^N\big)S_{-4}(N)$$

$$+ \Big(-\frac{2(-1)^N(9N+5)}{N(N+1)} - \frac{2}{N}\Big)S_{2,1}(N) + \big(20+2(-1)^N\big)S_{2,-2}(N) + \big(-17+13(-1)^N\big)S_{3,1}(N)$$

$$- \frac{8(-1)^N(2N+1)+4(9N+1)}{N(N+1)}S_{-2,1}(N) - \big(24+4(-1)^N\big)S_{-3,1}(N) + \big(3-5(-1)^N\big)S_{2,1,1}(N)$$

$$+ 32S_{-2,1,1}(N) + \left(\frac{3}{2}S_1(N)^2 - \frac{3S_1(N)}{N} + \frac{3}{2}(-1)^N S_{-2}(N)\right)\zeta(2)$$

$$S_1(N) = \sum_{i=1}^{N}\frac{1}{i}$$

$$S_2(N) = \sum_{i=1}^{N}\frac{1}{i^2}$$

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

$$\frac{7}{12}S_1(N)^4 + \frac{(17N+5)S_1(N)^3}{3N(N+1)} + \left(\frac{35N^2-2N-5}{2N^2(N+1)^2} + \frac{13S_2(N)}{2} + \frac{5(-1)^N}{2N^2}\right)S_1(N)^2$$

$$+\left(-\frac{4(13N \ldots}{N^2(N \ldots} \ldots N+1) \ldots 1) - \frac{13}{N}\right)S_2(N) + \left(\frac{29}{3} - (-1)^N\right)S_3(N)$$

$$+\left(2+2(-1)^{N} \ldots (N) + \frac{20(-1)^N}{N^2(N+1)}\right)S_1(N) + \left(\frac{3}{\ldots} \ldots\right.$$

$$-2(-1)^N S_{-2}(N)^2 + S_{-3}(N)\left(\frac{2(3N-5)}{N(N+1)} + (26+4(-1)^N)S_1(N) \ldots\right.$$

$$+\left(\frac{(-1)^N(5-3N)}{2N^2(N+1)} - \frac{5}{2N^2}\right)S_2(N) + S_{-2}(N)\left(10S_1(N)^2 + \left(\frac{8(-1 \ldots}{N(N+1)} \ldots\right.\right.$$

$$+\frac{4(3N-1)}{N(N+1)}\Big)S_1(N) + \frac{8(-1)^N(3N \ldots}{N(N+1 \ldots} \ldots \Big)$$

$$+\left(\frac{(-1)^N(9N+5)}{N(N+1)} - \frac{29}{3N}\right)S_3(N) + \ldots (N)$$

$$+\left(-\frac{2(-1)^N(9N+5)}{N(N+1)} - \frac{2}{N}\right)S_{2,1}(\ldots \ldots 1)^N\Big)S_{3,1}(N)$$

$$-\frac{8(-1)^N(2N+1)+4(9N+1)}{N(N+1)}S_{-\ldots} \ldots 1)^N\Big)S_{2,1,1}(N)$$

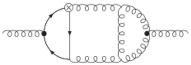
$$+32S_{-2,1,1}(N) + \left(\frac{3}{2}S_1(N)^2 - \frac{3S_1(N)}{N} + \frac{3}{2}(-1)^N S_{-2}(N)\right)\zeta(2)$$

$$S_1(N) = \sum_{i=1}^{N}\frac{1}{i}$$

$$S_2(N) = \sum_{i=1}^{N}\frac{1}{i^2}$$

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

Application: Evaluation of Feynman integrals



Behavior of particles $\longrightarrow$

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

Feynman integrals

$\Big\downarrow$ **DESY**

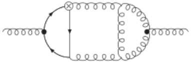
$$\sum f(N, \epsilon, k)$$

complicated multi-sums

$\xleftarrow[\text{(Sigma-package)}]{\textbf{advanced difference ring theory}}$

expression in special functions

Application: Evaluation of Feynman integrals



Behavior of particles

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

Feynman integrals

DESY

LHC at CERN

applicable

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

complicated
multi-sums

advanced difference ring theory

(Sigma-package)

expression in
special functions

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3. Logical Models of Problems and Computations

4. Modeling Problems in Geometry and Discrete Mathematics

- Problem 1: How to get from A to B?
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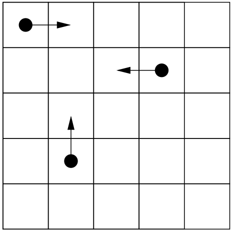
Example: A Robotic System

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 ⇔ R ≥ 1 ∧ P ≥ 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) ⇔
  ∀r1:Robot, r2:Robot with r1 < r2. x[r1] ≠ x[r2] ∨ y[r1] ≠ 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) ⇔ 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) ⇔
  ∃r0: Robot with r0 ≠ r. xr = x[r0] ∧ 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) ⇔
  (d = Left  ⇒ x[r] > 0   ∧ ¬anyOtherAt(x, y, r, x[r]-1, y[r]))
∧ (d = Right ⇒ x[r] < P-1 ∧ ¬anyOtherAt(x, y, r, x[r]+1, y[r]))
∧ (d = Up    ⇒ y[r] > 0   ∧ ¬anyOtherAt(x, y, r, x[r], y[r]-1))
∧ (d = Down  ⇒ y[r] < P-1 ∧ ¬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) ⇔
  ∃r:Robot, d:Direction with nextDir(x, y, r, d).
    x0 = moveX(x, r, d) ∧ y0 = moveY(y, r, d);

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

theorem _RobotsLogical_8_initPre_pverify_0(x:Positions, y:Positions)
⇔ ∀x0:Map[ℤ[0,2],ℤ[0,4]], y0:Map[ℤ[0,2],ℤ[0,4]]. (initialState(x0, y0) ⇒
    (letpar x = x0, y = y0 in noCollision(x, y)));
theorem _RobotsLogical_8_actionPre_0_pverify_0(x:Positions, y:Positions)
  requires noCollision(x, y);
⇔ ∀x0:Map[ℤ[0,2],ℤ[0,4]], y0:Map[ℤ[0,2],ℤ[0,4]].
    (nextState(x, y, x0, y0) ⇒ (letpar x = x0, y = y0 in noCollision(x, y)));
```

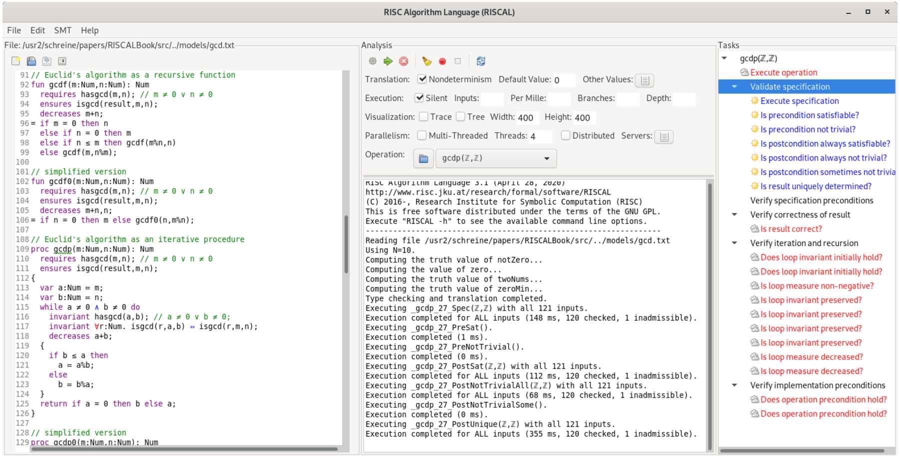
Course Contents

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



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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What is the mathematics behind navigation systems in modern cars?

Given: start address A, destination address B.

Find: “shortest route” from A to B.

Navigation Systems (trivial approach)

What is the mathematics behind navigation systems in modern cars?

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Find: "shortest route" from A to B.

Real world: A and B are given by geographical coordinates (2D or even 3D).

Navigation Systems (trivial approach)

What is the mathematics behind navigation systems in modern cars?

Given: start address A, destination address B.

Find: “shortest route” from A to B.

Real world: A and B are given by geographical coordinates (2D or even 3D).

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

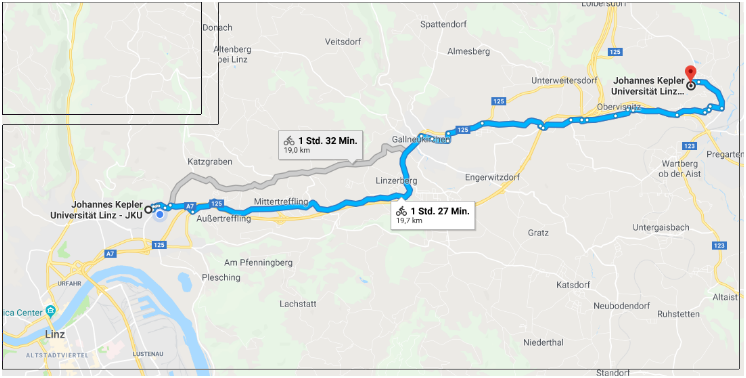
$$d_{\min} = \|B - A\|$$

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

Navigation Systems (realistic approach)

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

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



Navigation Systems (realistic approach)

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

Find: "shortest route" from A to B on S.

Mathematical model: Given n Streets S_i with $i = 1, \ldots, n$. 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 $V = \{C_{ij} \mid i, j = 1, \ldots, n\}$,
- adjacency relation between crossings $E = \{\{v_1, v_2\} \mid v_1 \text{ and } v_2 \text{ are adjacent}\}$,
- length of street segments $w \colon E \to \mathbb{R}^+$.

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
- $w\colon E \longrightarrow \mathbb{R}$.

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- $w : E \to \mathbb{R}$.

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

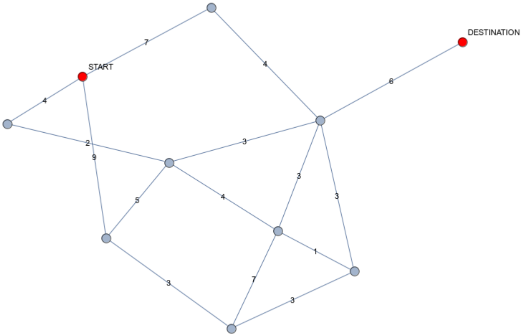
$$P_1 = A, P_n = B$$

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

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

Solution

The above problem is a well-known and well-studied problem in graph theory called the Shortest Path Problem.



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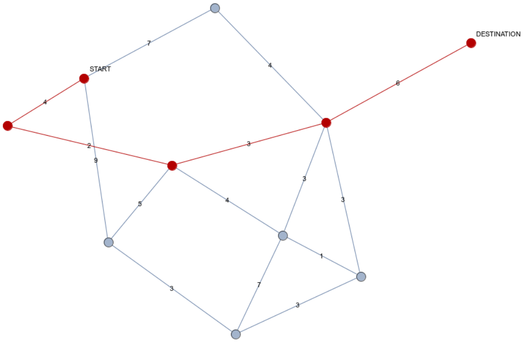

There are several algorithms to solve the Shortest Path Problem, e.g. Dijkstra's Algorithm or the Bellman-Ford-Algorithm.

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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- Production order does not play a role.
- 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 $O = \{1, \ldots, n\}$, duration $d\colon O \to \mathbb{R}$, stations $S = \{1, \ldots, m\}$, maximal operation time on stations $D\colon S \to \mathbb{R}$.

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

$$k \leq m, \tag{1}$$

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

$$\forall l < k \nexists t\colon O \to \{1, \ldots, l\} \forall j \in S : \sum_{\substack{i \in O \\ t(i)=j}} d(i) \leq D(j) \tag{3}$$

(2) means assignment obeys limit on every station.

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

Solution

The above problem is a well-known and well-studied problem in combinatorial optimization called the Bin Packing Problem.

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The above problem is a well-known and well-studied problem in combinatorial optimization called the Bin Packing Problem.

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.

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

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 exam: only 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.