

# Flyspeck II: The Basic Linear Programs 

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[^0]> To Frank Feuerstein,
> who was the first to teach me what mathematics is all about.

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## CHAPTER $\mathbf{1}$

## Introduction

There are two conflicting primal impulses of the human mind - one to simplify a thing to its essentials, the other to see through the essentials to the greater implications.

- Robert B. Laughlin

The Flyspeck project [14] has as its goal the complete formalization of Hales' proof $[15,16]$ of the Kepler conjecture which states that the best density one can hope for when packing infinitely many congruent balls is

$$
\frac{\pi}{\sqrt{18}} \approx 0.74
$$

The formalization has to be carried out within a mechanical theorem prover. For our work described in this thesis, we have chosen the interactive proof assistant Isabelle [25].

The proof of the Kepler conjecture proceeds in reducing the problem to a finite number of possible counter examples, the tame graphs. In a previous research effort [23], the enumeration of all tame graphs has been formalized and verified.

The final computational step of the Kepler conjecture is to prove by linear programming that all of these tame graphs cannot correspond to optimal packings, except those corresponding to the face-centered cubic or hexagonal-close packing.

In this thesis we focus on the basic linear programs, which are an important first milestone of taking this final step. With their help, we can eliminate 2565 of the 2771 tame graphs.

How reliable is this result? The major source of potential mayhem is that some mistake might have been introduced in the specification of the basic linear programs. The correctness of this specification will only be established after using the obtained results in the larger context of a complete formal proof of the Kepler conjecture. But even if there is such an error, we can console ourselves that the methods presented in this thesis are general enough so that a transfer to a corrected specification should be possible, and probably easy.

Another potential source of mistakes is the use of the HOL Computing Library
which we introduce and describe in the next chapter. After all, it is just a piece of unverified software which has been tested by only one person.

Apart from that, the usual claims of computer-checked proofs hold.

## CHAPTER 2

## The HOL Computing Library

Fast is fine, but accuracy is everything.

- Wyatt Earp


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### 2.1 What is the HCL?

The Higher-Order Logic Computing Library (HCL) is an extension of the Isabelle system [25] for fast and trusted computing. Work on it started in 2004 when it became clear that the Flyspeck project [14] demanded a flexible combination of computing power and theorem proving not available in the Isabelle system. HigherOrder Logic (HOL) contains a functional programming language; several research efforts have exposed and exploited this fact. Among these efforts has been to come
up with ever more powerful and clever packages for defining functions in this language [33], most recently the function package [19] in Isabelle. The major output of these packages is a list of proven equations about the defined functions which looks very much like a definition of these functions in a functional programming language like Standard ML (SML) [21, 29]. As you are working with a theorem prover, you would like to be able to execute those functions just like in SML, but with the goal of obtaining a theorem or parts of a theorem. Actually, you might want to do so for any list of proven equations which look like a functional program, no matter what their origin might be.

The established way of doing this in Isabelle is the Simplifier, which is a tool for doing trusted higher-order rewriting. How does the Simplifier gain your trust? By following a principle that the Edinburgh LCF theorem prover pioneered [9], and which also forms the heart of the Isabelle theorem prover. Theorems are represented as an abstract datatype, and the logic is encoded as operations on this abstract datatype. The Simplifier uses only those operations to generate and manipulate theorems. No matter how complex the implementation of the Simplifier is, all theorems that it generates are guaranteed to be correct as long as the abstract datatype of theorems is implemented correctly.

Obviously there is a price to pay for this combination of power and safety: performance. Compared to running an SML program, the Simplifier incurs a slowdown factor of 1000 and more. In many applications it is worth paying this price, but for the computations in this thesis such a performance penalty is prohibitive. The HCL closes this performance gap, so that computations resulting in theorems are possible with the speed of SML programs. Of course, there is again a price to pay for this performance increase: power and safety. The HCL is less powerful than the Simplifier: it has no congruence rules, but only weaker conditional rewrite rules, and there are no simplification procedures. Currently, the HCL is also not as safe as the Simplifier: there is no formal proof that the implementation of the HCL is correct, therefore you have to trust the HCL just as you trust the implementation of the abstract datatype of theorems. So when you use the HCL, you in fact view it as an extension of the trusted kernel of the Isabelle system. Assuming that the HCL has been implemented correctly, there is no way that using the HCL will produce incorrect theorems ${ }^{1}$.

### 2.2 Arithmetic in Commutative Rings with Unity

Arithmetic is the archetypal computational task and therefore a good first example for computing with the HCL. We choose the abstract setting of commutative rings with unity for doing arithmetic. We introduce an axiomatic type class Number which describes such rings. It assumes the presence of the familiar constants and axioms of ring theory (fig. 2.1). All these constants and axioms are polymorphic in $\alpha$, where $\alpha$ is a type variable of sort Number.

We also need a representation for numerals like 67. We adopt the standard approach of Isabelle which is based on [5] and choose a binary representation which can encode both positive and negative numbers. This has the advantage of a uniform addition algorithm which works for any combination of positive and negative operands. Such numerals are built up from four constants (fig. 2.2). Examples are

[^1]| Name | Type |
| :---: | :--- |
| Zero | $\alpha$ |
| One | $\alpha$ |
| add | $\alpha \rightarrow \alpha \rightarrow \alpha$ |
| mult | $\alpha \rightarrow \alpha \rightarrow \alpha$ |
| neg | $\alpha \rightarrow \alpha$ |


| add Zero $x$ | $=x$ |
| :--- | :--- |
| add $x y$ | $=$ add $y x$ |
| add (add $x y) z$ | $=$ add $x($ add $y z)$ |
| add (neg $x) x$ | $=$ Zero |
| mult One $x$ | $=x$ |
| mult $x y$ | $=$ mult $y x$ |
| mult $($ mult $x y) z$ | $=$ mult $x($ mult $y z)$ |
| mult $x($ add $y z)$ | $=\operatorname{add}($ mult $x y)($ mult $x z)$ |

Figure 2.1: Number Constants and Axioms

| Name | Type | Definition |
| :---: | :--- | :--- |
| Zero | $\alpha$ |  |
| Neg $_{1}$ | $\alpha$ | $N_{2}=$ neg One |
| $B_{0}$ | $\alpha \rightarrow \alpha$ | $B_{0} x=\operatorname{add} x x$ |
| $B_{1}$ | $\alpha \rightarrow \alpha$ | $B_{1} x=\operatorname{add}(\operatorname{add} x x)$ One |

Figure 2.2: Numeral Building Blocks
shown in Figure 2.3.
Negation is a little bit more difficult with this representation compared to a representation where you store the sign separately; it takes linear time instead of constant time. Linear-time addition is also a little bit tricky for the special case when you add two numerals which have both the shape $B_{1}(\ldots)$. An obvious solution seems to be

$$
\operatorname{add}\left(B_{1} x\right)\left(B_{1} y\right)=B_{0}(\operatorname{add}(\operatorname{add} x y) \text { One })
$$

but it is not clear that this is a linear-time rule as computing the successor is worstcase linear-time itself which could lead to a quadratic-time rule for add. We define two helper functions neg ${ }_{1}$ and $a d d_{1}$ to deal with these difficulties:

$$
\begin{array}{ll}
\operatorname{neg}_{1} x & =\text { neg (add } x \text { One }) \\
\operatorname{add}_{1} x y & =\text { add (add } x y) \text { One. }
\end{array}
$$

It is then straightforward to prove theorems about negation (fig. 2.4), addition (fig. 2.5) and multiplication (fig. 2.6) which actually look like a functional program for computing these operations on numerals. There are also theorems for normalizing numerals (fig. 2.7).

| Decimal | Binary | Numeral |
| :---: | :---: | :--- |
| 0 | 0 | Zero |
| 1 | 1 | $B_{1}$ Zero |
| -1 | -1 | Neg |
| 2 | 10 | $B_{0}\left(B_{1}\right.$ Zero $)$ |
| -2 | -10 | $B_{0}$ Neg $_{1}$ |
| 67 | 1000011 | $B_{1}\left(B_{1}\left(B_{0}\left(B_{0}\left(B_{0}\left(B_{0}\left(B_{1}\right.\right.\right.\right.\right.\right.$ Zero $\left.\left.\left.\left.\left.)\right)\right)\right)\right)\right)$ |
| -67 | -1000011 | $B_{1}\left(B_{0}\left(B_{1}\left(B_{1}\left(B_{1}\left(B_{1}\left(B_{0}\right.\right.\right.\right.\right.\right.$ Neg 1$\left.\left.\left.\left.\left.)\right)\right)\right)\right)\right)$ |

Figure 2.3: Numeral Examples
neg Zero $=$ Zero
neg Neg $=B_{1}$ Zero
neg $\left(B_{0} x\right)=B_{0}($ neg $x)$
neg $\left(B_{1} x\right)=B_{1}\left(n_{1} x\right)$

| neg $_{1}$ Zero | $=$ Neg $_{1}$ |
| ---: | :--- |
| neg $_{1}$ Neg $_{1}$ | $=$ Zero |
| neg $_{1}\left(B_{0} x\right)$ | $=B_{1}\left(\right.$ neg $\left._{1} x\right)$ |
| neg $_{1}\left(B_{1} x\right)$ | $=B_{0}\left(\right.$ neg $\left._{1} x\right)$ |

Figure 2.4: Computing Negation

| add $\left(B_{0} x\right)\left(B_{0} y\right)$ | $B_{0}($ add $x y)$ | $\operatorname{add}_{1}\left(B_{0} x\right)\left(B_{0} y\right)$ | $B_{1}($ add $x y)$ |
| :---: | :---: | :---: | :---: |
| add $\left(B_{0} x\right)\left(B_{1} y\right)$ | $B_{1}(\operatorname{add} x y)$ | $\operatorname{add}_{1}\left(B_{0} x\right)\left(B_{1} y\right)$ | $B_{0}\left(\operatorname{add}_{1} x y\right)$ |
| add ( $\left.B_{1} x\right)\left(B_{0} y\right)$ | $B_{1}(\operatorname{add} x y)$ | $\operatorname{add}_{1}\left(B_{1} x\right)\left(B_{0} y\right)$ | $B_{0}\left(\operatorname{add}_{1} x y\right)$ |
| add ( $\left.B_{1} x\right)\left(B_{1} y\right)$ | $B_{0}\left(\operatorname{add}_{1} x y\right)$ | $\operatorname{add}_{1}\left(B_{1} x\right)\left(B_{1} y\right)$ | $B_{1}\left(\operatorname{add}_{1} x y\right)$ |
| add Zero $x$ | $=x$ | $\operatorname{add}_{1} \mathrm{Neg}_{1} x$ | $x$ |
| add $x$ Zero | $=x$ | $\operatorname{add}_{1} \times \mathrm{Neg}_{1}$ | $x$ |
| add $\operatorname{Neg}_{1}\left(B_{0} x\right)$ | $B_{1}\left(\operatorname{add} \operatorname{Neg}_{1} x\right)$ | $\operatorname{add}_{1}$ Zero ( $B_{0} x$ ) | $B_{1} x$ |
| add $\operatorname{Neg}_{1}\left(B_{1} x\right)$ | $B_{0} x$ | $\operatorname{add}_{1}$ Zero ( $B_{1} x$ ) | $B_{0}\left(\right.$ add $_{1}$ Zero $\left.x\right)$ |
| add ( $\left.B_{0} x\right) \mathrm{Neg}_{1}$ | $B_{1}\left(\right.$ add $\left.x \mathrm{Neg}_{1}\right)$ | $\operatorname{add}_{1}\left(B_{0} x\right)$ Zero | $B_{1} x$ |
| add ( $\left.B_{1} x\right) \mathrm{Neg}_{1}$ | $=B_{0} x$ | $\operatorname{add}_{1}\left(B_{1} x\right)$ Zero | $B_{0}\left(\right.$ add $_{1} \times$ Zero $)$ |
| add $\mathrm{Neg}_{1} \mathrm{Neg}_{1}$ | $=B_{0} \mathrm{Neg}_{1}$ | $\operatorname{add}_{1}$ Zero Zero | $B_{1}$ Zero |

Figure 2.5: Computing Addition

```
mult x Zero = Zero
mult Zero x = Zero
mult Neg
mult x Neg1 = neg x
mult (B0 x) y = B (mult x y)
mult x (B0y) = B (mult x y)
mult (B1 x) (B1y) = B B (add (B0 (mult x y )) (add x y ))
```

Figure 2.6: Computing Multiplication

$$
\begin{aligned}
& B_{0} \text { Zero }=\text { Zero } \\
& B_{1} \text { Neg }_{1}=\text { Neg }_{1}
\end{aligned}
$$

Figure 2.7: Normalizing Numerals
signature NUMERAL = sig
signature NUMERAL = sig
datatype Numeral = Zero | Neg1
datatype Numeral = Zero | Neg1
| BO of Numeral | B1 of Numeral
| BO of Numeral | B1 of Numeral
val neg : Numeral -> Numeral
val neg : Numeral -> Numeral
val add : Numeral -> Numeral -> Numeral
val add : Numeral -> Numeral -> Numeral
val mult : Numeral -> Numeral -> Numeral
val mult : Numeral -> Numeral -> Numeral
val norm : Numeral -> Numeral
val norm : Numeral -> Numeral
val test : Numeral -> bool
val test : Numeral -> bool
val fac : Numeral -> Numeral
val fac : Numeral -> Numeral
end
end
structure Numeral : NUMERAL = struct
structure Numeral : NUMERAL = struct
datatype Numeral = Zero | Neg1
datatype Numeral = Zero | Neg1
| B0 of Numeral | B1 of Numeral
| B0 of Numeral | B1 of Numeral
fun add ( $B Q x$ ) ( $B Q y$ ) $=B Q$ (add $x y)$
fun add ( $B Q x$ ) ( $B Q y$ ) $=B Q$ (add $x y)$
$\mid$ add (B0 x) (B1 y) = B1 (add $x y)$
$\mid$ add (B0 x) (B1 y) = B1 (add $x y)$
$\mid \operatorname{add}(B 1 x)(B Q y)=B 1(a d d x y)$
$\mid \operatorname{add}(B 1 x)(B Q y)=B 1(a d d x y)$
$\mid$ add (B1 x) (B1 y) = B0 (add1 x y)
$\mid$ add (B1 x) (B1 y) = B0 (add1 x y)
| add Zero $\mathrm{x}=\mathrm{x}$
| add Zero $\mathrm{x}=\mathrm{x}$
| add x Zero $=\mathrm{x}$
| add x Zero $=\mathrm{x}$
| add Neg1 (BO x) = B1 (add Neg1 x)
| add Neg1 (BO x) = B1 (add Neg1 x)
| add Neg1 (B1 x) = BO x
| add Neg1 (B1 x) = BO x
| add (B0 x) Neg1 = B1 (add $x$ Neg1)
| add (B0 x) Neg1 = B1 (add $x$ Neg1)
| add (B1 x) Neg1 = BO x
| add (B1 x) Neg1 = BO x
| add Neg1 Neg1 = B0 Neg1
| add Neg1 Neg1 = B0 Neg1
and add1 ( $B Q x$ ) ( $B \cap y$ ) $=B 1$ (add $x y)$
and add1 ( $B Q x$ ) ( $B \cap y$ ) $=B 1$ (add $x y)$
$\mid$ add1 ( BQ x ) ( B 1 y ) $=\mathrm{BQ}$ (add1 $\mathrm{x} y)$
$\mid$ add1 ( BQ x ) ( B 1 y ) $=\mathrm{BQ}$ (add1 $\mathrm{x} y)$
| add1 (B1 x) (B0 y) = BO (add1 x y)
| add1 (B1 x) (B0 y) = BO (add1 x y)
| add1 (B1 x) (B1 y) = B1 (add1 x y)
| add1 (B1 x) (B1 y) = B1 (add1 x y)
| add1 Neg1 $\mathrm{x}=\mathrm{x}$
| add1 Neg1 $\mathrm{x}=\mathrm{x}$
| add1 x Neg1 = x
| add1 x Neg1 = x
| add1 Zero (BO x) = B1 x
| add1 Zero (BO x) = B1 x
| add1 Zero (B1 x) = B0 (add1 Zero x)
| add1 Zero (B1 x) = B0 (add1 Zero x)
| add1 (B0 x) Zero = B1 x
| add1 (B0 x) Zero = B1 x
| add1 (B1 x) Zero = B0 (add1 x Zero)
| add1 (B1 x) Zero = B0 (add1 x Zero)
| add1 Zero Zero = B1 Zero
| add1 Zero Zero = B1 Zero
fun neg Zero = Zero
| neg Neg1 = B1 Zero
$\mid \operatorname{neg}(B 0 x)=B 0(n e g x)$
| neg (B1 x) $=$ B1 (neg1 $x$ )
and neg1 Zero $=$ Neg1
| neg1 Neg1 = Zero
| neg1 (BO x) = B1 (neg1 x)
$\mid \operatorname{neg} 1(B 1 x)=B 0(n e g 1 x)$
fun mult x Zero = Zero
| mult Zero $x=$ Zero
| mult Neg1 $x=n e g x$
| mult x Neg1 = neg x
| mult (BQ x) y = BQ (mult $x y$ )
| mult $x$ ( $B Q y$ ) $=B Q$ (mult $x y$ )
| mult (B1 x) (B1 y) =
B1 (add (B0 (mult $x$ y)) (add $x y)$ )
fun norm Zero = Zero
| norm Neg1 = Neg1
| norm (BO x) =
(case norm $x$ of
Zero => Zero
| x => BQ x)
$\mid \operatorname{norm}(\mathrm{B} 1 \mathrm{x})=$
(case norm $x$ of
Neg1 => Neg1
| x => B1 x )
fun test Zero = true
| test Neg1 = false
| test (BO x) = test $x$
| test (B1 x) = false
fun fac $\mathrm{n}=$
if test n then
B1 Zero
else
mult n (fac (add n Neg1))
end

Figure 2.8: Standard ML Module for Computing with Numerals

### 2.3 Performance Showdown: Factorials

We will now apply both the HCL and the Simplifier of Isabelle to the problem of computing factorials using the list $L$ of theorems displayed in Figures 2.4, 2.5, 2.6 and 2.7. Both HCL and Simplifier can be used as functions from $L$ to a conversion. This conversion is a function taking a term $t$ and returning a theorem $t=F t$, where $F t$ is the result of rewriting $t$ according to $L$. To assess the performance of the HCL and the Simplifier we will be looking at a whole family $t_{i}$ of polymorphic terms where

$$
t_{0}=N_{1} \quad \text { and } \quad t_{i+1}=\text { mult }_{i} N_{i+1} .
$$

The term $N_{i}$ is the numeral corresponding to $i$, e.g. $N_{1}=B_{1}$ (Zero :: $\alpha::$ Number), such that it cannot be rewritten further using the theorems in Figure 2.7. In other words, we request that $N_{i}$ be normalized.

Applying the conversion to $t_{i}$ will yield the theorem

$$
t_{i}=N_{i!} .
$$

We admit one more competitor to this contest: Standard ML itself. The list $L$ looks almost like a functional program, and it is easy to convert it into a true Standard ML program (fig. 2.8). All we need to do is to

1. introduce an SML datatype Numeral consisting of four constructors corresponding to the constants Zero, Neg ${ }_{1}, B_{0}$ and $B_{1}$,
2. introduce SML functions neg, add and mult (together with their helper functions) which correspond to the constants neg, add and mult, and which behave according to Figures 2.4, 2.5, 2.6,
3. introduce an SML function norm which does the normalization according to Figure 2.7. There is no Isabelle constant norm to which norm corresponds, as logically, norm would just be the identity.

Additionally, there is a function test which checks if the normalization of its input yields Zero ${ }^{2}$, and there is a function fac which calculates the factorial of its input using test. Let $N_{i}$ be the SML version of $N_{i}$, then Standard ML enters the contest by computing norm (fac $\mathrm{N}_{i}$ ).

The results of the performance showdown are summarized in Tables 2.1 and 2.2. The measurements have been taken on an Intel Core2 Duo 2.0 GHz processor running Isabelle 2007 / PolyML 5.0 / GHC 6.6.1. Missing entries in the tables do not indicate nontermination but just that these measurements have not been taken.

Table 2.1 displays the total runtime of each method, while Table 2.2 displays the slowdown factor of how many times slower each method worked relative to just running a functional program. This slowdown factor grows rapidly with the size of the computation for the Simplifier, but it remains constant or even improves for the HCL. The HCL can be operated in different modes. The Barras mode performs interpreted evaluation while both the Haskell mode and the SML mode perform compiled evaluation. The slowdown factor for the Barras mode seems to be between 130 and 90, converging to the better end of this spectrum for large inputs. The Haskell mode uses the external Glasgow Haskell compiler and has therefore huge

[^2]| i | Simplifier | HCL (Barras) compu | HCL (Haskell) ing theorem $=N_{i}$ ! | HCL (SML) | Standard ML computing SML value norm (fac $\mathrm{N}_{i}$ ) |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 10 | 0.0026 | 0.0008 | 0.37 | 0.00048 | 0.000006 |
| 20 | 0.016 | 0.0026 | 0.38 | 0.00095 | 0.000023 |
| 40 | 0.123 | 0.013 | 0.4 | 0.0019 | 0.00012 |
| 80 | 1.18 | 0.072 | 0.45 | 0.0048 | 0.0008 |
| 160 | 13.1 | 0.4 | 0.54 | 0.0143 | 0.0041 |
| 320 | 151 | 2.3 | 0.8 | 0.047 | 0.024 |
| 640 | 1514 | 12.4 | 1.74 | 0.2 | 0.13 |
| 1280 | 16400 | 64.8 | 5.5 | 0.91 | 0.71 |
| 2560 | - | 333 | 22.5 | 4.47 | 3.59 |
| 5120 | - | 1655 | 102 | 22.5 | 18.7 |
| 10240 | - | - | 508 | 105 | 102 |
| 20480 | - | - | - | 593 | 576 |

Table 2.1: Performance Showdown (runtime in seconds)

| $i$ | Simplifier | HCL (Barras) compu | HCL (Haskell) <br> ing theorem $=N_{i}$ ! | HCL (SML) | Standard ML computing SML value norm (fac $\mathrm{N}_{i}$ ) |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 10 | 433 | 133 | 61667 | 80 | 1 |
| 20 | 696 | 113 | 16521 | 41 | 1 |
| 40 | 1025 | 108 | 3333 | 16 | 1 |
| 80 | 1475 | 90 | 563 | 6 | 1 |
| 160 | 3195 | 97 | 38 | 3.5 | 1 |
| 320 | 6291 | 96 | 17 | 2 | 1 |
| 640 | 11646 | 95 | 13 | 1.5 | 1 |
| 1280 | 23099 | 91 | 8 | 1.3 | 1 |
| 2560 | - | 93 | 5 | 1.2 | 1 |
| 5120 | - | 89 | 5.5 | 1.2 | 1 |
| 10240 | - | - | 5 | 1.03 | 1 |
| 20480 | - | - | - | 1.03 | 1 |

Table 2.2: Performance Showdown ( $\left.\frac{\text { runtime of method }}{\text { runtime for computing SML value }}\right)$

| test-le Zero | $=$ True | test-less Zero | $=$ False |
| :--- | :--- | :--- | :--- |
| test-le Neg | $=$ True | test-less Neg | $=$ True |
| test-le $\left(B_{0} x\right)$ | $=$ test-le $x$ | test-less $\left(B_{0} x\right)$ | $=$ |
| test-less $x$ |  |  |  |
| test-le $\left(B_{1} x\right)$ | $=$ test-less $x$ | test-less $\left(B_{1} x\right)$ | $=$ test-less $x$ |

Figure 2.9: Signs of Integer Numerals
overhead. For long computations though its slowdown factor converges to 5. For the SML mode the numbers are even better: although for small inputs due to noncomputational overhead the slowdown factor can be around 80 , too, the situation improves dramatically for larger inputs, approaching 1.2 for computations which last a few seconds, and even approaching 1.03 for computations which last minutes.

The road to theorem proving performance that rivals the performance of functional programs is therefore clear: use computing libraries like the HCL, and package computation in as large chunks as possible to avoid the large slowdown factors for small inputs.

### 2.4 Controlling Evaluation

The observant reader might have noticed that for our performance showdown in the previous section we had an SML function fac for computing the factorial of a Numeral but no corresponding Isabelle constant fac. Instead we worked with an explicit product. This was not really important for the showdown because the computational difference is only slight, but in order to explain some issues concerning the evaluation strategy employed by the HCL, we now introduce such a constant.

However, our current general setting of commutative rings poses difficulties for defining and executing fac. A definition like

$$
\text { fac } x=\text { if } x=\text { Zero then } B_{1} \text { Zero else mult } x\left(\text { fac }\left(\operatorname{add} x \operatorname{Neg}_{1}\right)\right)
$$

would render fac in most rings a partial function, which is inconvenient as HOL is a logic of total functions. While this problem could be solved using the function package [19] for definining partial functions, there is a more serious one. Just based on the axioms from Figure 2.1 we cannot devise an executable test if a ring numeral is equal to Zero or not, which is clearly a prerequisite for executing the above specification. For example, the equation $B_{0}\left(B_{1}\right.$ Zero $)=$ Zero holds for any field of characteristic 2 , but is false for the ring of integers.

To simplify matters, we therefore leave the general setting of rings and look at the specific setting of the ring of integers. Here it is no problem to define a total function which is constant on negative integers and which behaves like the factorial function on nonnegative integers:

$$
\begin{equation*}
\text { fac } x=\text { if test-le } x \text { then } B_{1} \text { Zero else mult } x\left(\text { fac }\left(\operatorname{add} x \operatorname{Neg}_{1}\right)\right) \tag{2.1}
\end{equation*}
$$

The function test-le checks if its argument is less than or equal to Zero. The theorems for executing it are listed in Figure 2.9. So how do we execute fac?

### 2.4.1 Conditional Rules

Until now all theorems we gave to the HCL had the form of equations. Actually, the HCL accepts theorems that have a more general shape:

$$
\begin{equation*}
A_{1} \equiv B_{1} \Longrightarrow \ldots \Longrightarrow A_{m} \equiv B_{m} \Longrightarrow f p_{1} p_{2} \ldots p_{n} \equiv T \tag{2.2}
\end{equation*}
$$

The symbols $\equiv$ and $\Longrightarrow$ denote Isabelle's meta notions of equality and implication, respectively. Furthermore, $f p_{1} p_{2} \ldots p_{n}$ must be a linear pattern, but $f$ may not be a variable.

## A pattern is either

## 1. a variable

2. or a term of the form $f p_{1} p_{2} \ldots p_{n}$, such that $f$ is a constant and all $p_{i}$ are patterns.

A pattern is called linear if no variable occurs more than once in it.
Each variable occurring free in $T$ or in any of the $A_{j}$ or $B_{j}$ must occur in one of the patterns.

Such a rule instructs the HCL to rewrite a term $f q_{1} q_{2} \ldots q_{n}$ by first matching each $q_{i}$ to the corresponding $p_{i}$. If this does not succeed then the rule is ignored. If the matching succeeds then each of the variables in the patterns will be bound. Substituting these variables in $T$ and in each $A_{j}$ and $B_{j}$ results in $T^{\prime}, A_{j}^{\prime}$ and $B_{j}^{\prime}$. Afterwards the $A_{j}^{\prime}$ and $B_{j}^{\prime}$ are evaluated by the HCL, resulting in $A_{j}^{\prime \prime}$ and $B_{j}^{\prime \prime}$. If for all $j$ the terms $A_{j}^{\prime \prime}$ and $B_{j}^{\prime \prime}$ are structurally equal, then $f q_{1} q_{2} \ldots q_{n}$ is replaced by $T^{\prime}$, otherwise the rule is ignored.

Therefore, one way of telling the HCL how to execute fac is through conditional rules:

$$
\begin{aligned}
& \text { test-le } x \longrightarrow \\
& \text { fac } x=B_{1} \text { Zero, } \\
& \neg \text { test-le } x \longrightarrow \\
& \text { fac } x=\text { mult } x\left(\text { fac }\left(\text { add } x \text { Neg }_{1}\right)\right) .
\end{aligned}
$$

These two rules can be mechanically transformed into

$$
\begin{aligned}
\text { test-le } x \equiv \text { True } & \Longrightarrow \quad \text { fac } x \equiv B_{1} \text { Zero } \\
(\neg \text { test-le } x) \equiv \text { True } & \Longrightarrow \quad \text { fac } x \equiv \operatorname{mult} x\left(\text { fac }\left(\text { add } x \operatorname{Neg}_{1}\right)\right)
\end{aligned}
$$

to match the description of rules accepted by the HCL given above.

### 2.4.2 Strict or Lazy Evaluation?

Instead of splitting the definition of fac into two conditional rules it seems more natural to use its definition directly. This raises the question of how to execute the if-then-else construct in (2.1). The HCL has no special built-in support for this construct; to it, it is just another function If taking three arguments. Therefore we have to provide equations which express the behavior of this If constant:

$$
\begin{align*}
\text { If True } a b & =a \\
\text { If False } a b & =b \tag{2.3}
\end{align*}
$$

The evaluation of fac Zero could then successfully proceed as follows:

```
fac Zero
    \(\equiv \quad\) if test-le Zero then \(B_{1}\) Zero else mult Zero (fac (add Zero Neg \({ }_{1}\) ))
    \(\equiv \quad\) if True then \(B_{1}\) Zero else mult Zero (fac (add Zero Neg \({ }_{1}\) ))
    \(\equiv \overline{B_{1} \text { Zero }}\)
```

Here is a legal, but not terminating evaluation:

```
fac Zero
    \(\equiv \quad\) if test-le Zero then \(B_{1}\) Zero else mult Zero (fac (add Zero Neg \(\left._{1}\right)\) )
    \(\equiv \quad\) if test-le Zero then \(B_{1}\) Zero else mult Zero (fac \(\overline{\mathrm{Neg}_{1}}\) )
    \(\equiv \quad\) if test-le Zero then \(B_{1}\) Zero
    else mult Zero (if test-le \(N e g_{1}\) then \(B_{1}\) Zero else mult \(\mathrm{Neg}_{1}\left(\right.\) fac (add \(\left.N e g_{1} N e g_{1}\right)\) ))
    \(\equiv \quad\) if test-le Zero then \(B_{1}\) Zero
        else mult Zero (if test-le \(N e g_{1}\) then \(B_{1}\) Zero else mult \(\operatorname{Neg}_{1}\left(f a c\left(B_{0} N e g_{1}\right)\right)\) )
    \(\equiv\)
```

Which evaluation path will the HCL take? One of the above, or maybe even another, third one?

Actually, this depends on the mode of the HCL. As mentioned earlier, there are different modes of the HCL, most prominently the Barras mode, the SML mode, and the Haskell mode. The Haskell mode performs lazy evaluation and will therefore find a terminating path for evaluating fac Zero. Both the Barras and the SML mode evaluate all the arguments that are mentioned on the left hand side of a rule before applying the rule, and will therefore diverge.

The trouble is that depending on the value of the first argument of If either the second or the third argument should not be evaluated. There is a way to teach the HCL this special evaluation strategy. If both the Barras and the SML mode need to evaluate all the arguments on the left hand side of a rule before applying the rule, but you do not want the last two arguments of If to be evaluated prematurely, then just remove these two arguments from the left hand side and move them to the right hand side!

Applying this to the equations (2.3) yields new equations for If which mark the first argument as strict and the last two arguments as lazy:

$$
\begin{align*}
\text { If True } & =\lambda a b \cdot a \\
\text { If False } & =\lambda a b \cdot b \tag{2.4}
\end{align*}
$$

The reasons why this results in the behavior we wish for depend again on the mode. For the Haskell mode, everything has worked before and will continue to work. For the Barras mode and the SML mode special care has been taken to accommodate the desired behavior. For details on this see the later sections which describe the implementation of each mode.

Note that this method allows us to split the $n=n_{\text {strict }}+n_{\text {lazy }}$ arguments of any function into two groups. The first group is made up of the first $n_{\text {strict }}$ arguments which are evaluated strictly. The second group is made up of the last $n_{\text {lazy }}$ arguments which are evaluated lazily. The Barras mode is more general than the SML mode in that it allows this grouping to vary from rule to rule. In the SML mode it is assumed that there is a fixed grouping for all rules which belong to the same function.

Another, albeit related, application of this feature is to implement short-circuit boolean operators, listed in Figure 2.10. The operators given there are defined using the already available corresponding logical operators of Isabelle/HOL. There is no


Figure 2.10: Short-circuit Boolean Operators of Type bool $\rightarrow$ bool $\rightarrow$ bool
need to define new operators to obtain a different evaluation strategy for existing operators. But in doing so we are able to use different evaluation strategies at the same time.

It is a strength of our approach that via modes pure computing is decoupled from the embedding into a theorem proving environment. The HCL is easily extendable this way. Do you wish that the HCL could evaluate all arguments of a function in parallel? Then just implement a mode that has this feature. Or outsource this task to somebody who is an expert in programming parallel compilers but maybe has no clue about theorem proving.

### 2.5 Modes of the HCL

So what exactly is a mode of the HCL? It is an implementation of the abstract machine interface we describe in this section.

Expressions in a theorem prover are complicated. There are terms, types embedded in and describing those terms, theorems, sorts of types, assumptions of theorems, meta assumptions of theorems and so on. To deal correctly with these complications is not trivial and mistakes are easily introduced if one handles them directly bypassing the protective layer of the theorem prover kernel. The design of the HCL takes this potential source of mistakes into account and separates the administrative tasks of the computing library from the actual task of computing. The administrative branch of the HCL supports major features of Isabelle like axiomatic type classes, polymorphism, overloading and locales, and will be studied later. In this section we look at our interface for raw computing and at two of its implementations, the Barras mode and the SML mode. There is also a Haskell mode which is similar to the SML mode, and we will mention some of the differences.

### 2.5.1 An Abstract Machine Interface

Each computing mode can be viewed as a black box. You give it a program and a term, and the black box will return another term which is the result of running the input program on the input term. This black box is what we call our abstract machine. To describe it, we need to explain how exactly our terms and programs look like, and what it means to run such programs on such terms.

An abstract machine term is inductively defined via

$$
\text { term }::=\operatorname{Var} v \mid \text { Const } c \mid \text { term }_{1} \cdot \text { term }_{2} \mid \lambda \text { term } \mid \text { Computed term }
$$

4 Definition 2.2
Abstract Machine Term
such that $v \in \mathbb{N}$ and $c \in \mathbb{Z}$. A pure term is one that does not contain any Computed terms.

An abstract machine term is just a $\lambda$ calculus term in de Bruijn index notation [6], with constants and with an additional constructor Computed. For specification purposes Computed $t$ can be treated just like $t$; it is a hint for the abstract machine implementation that $t$ has already been computed and needs no further processing. The implementation may ignore this hint.

When we write $t_{1}=t_{2}$ for two abstract machine terms $t_{1}$ and $t_{2}$ we are referring to the equality naturally arising from the inductive definition of terms.The advantage of using de Bruijn indices is that we do not need to concern ourselves with $\alpha$ equivalence of $\lambda$ terms.

Definition $2.3-A n$ abstract machine pattern is inductively defined via

Abstract Machine Pattern

Definition 2.4 checkfrees

$$
\text { pattern }::=P \operatorname{Var} \mid P \text { Const } c\left[\text { pattern }_{1}, \ldots, \text { pattern }_{n}\right]
$$

such that $c \in \mathbb{Z}$.

We denote the number of occurrences of $P$ Var in a pattern $p$ by $|p|$. An abstract machine pattern is just a compact encoding of certain abstract machine terms. Let us denote the term that corresponds to a given pattern $p$ by $[p]_{T}$ :

$$
\begin{aligned}
{ }_{[p]_{T}} & =[p]_{T, 0} \\
{[P \operatorname{Var}]_{T, i} } & =\operatorname{Var} i \\
{\left[P C o n s t c\left[p_{1}, \ldots, p_{n}\right]\right]_{T, i} } & =\left(\ldots\left(\left((\text { Const } c) \cdot q_{1}\right) \cdot q_{2}\right) \cdots\right) \cdot q_{n} \\
\text { where } q_{j} & =\left[p_{j}\right]_{T, I(j)} \text { and } I(j)=i+\sum_{k=j+1}^{n}\left|p_{k}\right|
\end{aligned}
$$

So $[p]_{T}$ arises from $p$ in the obvious way by enumerating the variables from right to left.

The idea is that a pair $(p, t)$ of a pattern $p$ and a term $t$ induces a rewrite rule $[p]_{T}=t$. We also require that in such a rewrite rule any free variable in $t$ must be bound by $p$.

$$
\begin{array}{ll}
\text { checkfrees } f(\text { Var } v) & =v<f \\
\text { checkfrees } f(\text { Const }) & =\text { true } \\
\text { checkfrees } f\left(t_{1} \cdot t_{2}\right) & =\text { checkfrees } f t_{1} \wedge \text { checkfrees } f t_{2} \\
\text { checkfrees } f(\lambda t) & =\text { checkfrees }(f+1) t \\
\text { checkfrees } f(\text { Computed } t) & =\text { checkfrees } f t
\end{array}
$$

The requirement that in a rewrite rule $[p]_{T}=t$ any free variable in $t$ must be bound by $p$ can be expressed with the formula checkfrees $|p| t$.

Definition 2.5 Abstract Machine Program

An abstract machine rule is a triple $\left(\left[\left(a_{1}, b_{1}\right), \ldots,\left(a_{n}, b_{n}\right)\right], p, t\right)$ such that

1. $p$ is an abstract machine pattern and $p \neq P$ Var,
2. $t$ is a pure abstract machine term,
3. checkfrees $|p| t$ holds,
4. the $a_{i}$ and $b_{i}$ are pure abstract machine terms with checkfrees $|p| a_{i}$ and checkfrees $|p| b_{i}$, respectively. The pairs $\left(a_{i}, b_{i}\right)$ are called guards.

An abstract machine program is a list of abstract machine rules.

Now that we know what an abstract machine program looks like, how does it operate on a term? Although we assume familiarity with de Bruijn indices [6] and the $\lambda$ calculus, we will first define $\beta$ reduction and related notions for abstract machine terms so that we have the complete definition of the abstract machine interface in one place.
$(\operatorname{Var} v) \uparrow^{n} \quad= \begin{cases}\operatorname{Var} v & \text { if } v<n \\ \operatorname{Var}(v+1) & \text { if } v \geq n\end{cases}$

4 Definition 2.6 Lifting

- Definition 2.7 Lowering

Let now $\zeta$ be a substitution, i.e. a partial function from $\mathbb{N}$ to abstract machine terms. The substitution $\zeta \uparrow$ is then defined by

$$
(\zeta \uparrow) v= \begin{cases}\text { undefined } & \text { if } v=0 \text { or } v>0 \wedge \zeta(v-1) \text { is undefined } \\ \zeta(v-1) \uparrow^{0} & \text { if } v>0 \wedge \zeta(v-1) \text { is defined }\end{cases}
$$

$(\operatorname{Var} v)[\zeta] \quad= \begin{cases}\zeta v & \text { if } \zeta v \text { is defined } \\ \operatorname{Var} v & \text { if } \zeta v \text { is undefined }\end{cases}$
4 Definition 2.8 Substitution
•Definition 2.9
5. Computed $t \rightarrow_{\beta}$ Computed $t^{\prime}$ if $t \rightarrow_{\beta} t^{\prime}$

Lowering is actually a partial function because e.g. ( $\operatorname{Var} 0) \downarrow_{0}$ is not defined; but we use it in the definition of $\beta$ reduction only on an argument for which it is defined.

By defining $\beta$ reduction we put one aspect of computing in place. On top of it we can build the other aspect, which is how to make use of the rules of an abstract machine program. For this we define $\tau$ reduction. When talking about $\tau$ reduction, we always have some specific abstract machine program in mind which does not appear explicitly in our notation but should be clear from the context.

Definition 2.10 * $\tau$ Reduction

1. $t_{1} \Rightarrow_{\tau} t_{2}$ if $t_{1} \rightarrow_{\tau}^{*} t_{2}$
2. $t_{1}={ }_{\tau} t_{2}$ if $\exists s . t_{1} \Rightarrow_{\tau} s \wedge t_{2} \Rightarrow_{\tau} s$
3. $\zeta$ is a substitution
4. $\quad\left([p]_{T}\right)[\zeta] \rightarrow_{\tau} t[\zeta] \quad$ if $\quad$ 2. and $\left(\left[\left(a_{1}, b_{1}\right), \ldots,\left(a_{n}, b_{n}\right)\right], p, t\right)$ is a rule of the program
5. and $a_{i}[\zeta]={ }_{\tau} b_{i}[\zeta]$ for all $i=1, \ldots, n$
6. $t \rightarrow_{\tau} t^{\prime} \quad$ if $\quad t \rightarrow_{\beta} t^{\prime}$ or $t^{\prime} \rightarrow_{\beta} t \quad(\beta$ conversion)
7. $\quad t \rightarrow{ }_{\tau} \lambda\left(t \uparrow^{0} \cdot \operatorname{Var} 0\right)$ and $\lambda\left(t \uparrow^{0} \cdot \operatorname{Var} 0\right) \rightarrow_{\tau} t \quad$ ( $\eta$ conversion)
8. $\lambda t \rightarrow_{\tau} \lambda t^{\prime}$ if $t \rightarrow_{\tau} t^{\prime}$
9. $t_{1} \cdot t_{2} \rightarrow_{\tau} t_{1}^{\prime} \cdot t_{2} \quad$ if $t_{1} \rightarrow_{\tau} t_{1}^{\prime}$
10. $t_{1} \cdot t_{2} \rightarrow_{\tau} t_{1} \cdot t_{2}^{\prime} \quad$ if $t_{2} \rightarrow_{\tau} t_{2}^{\prime}$
11. Computed $t \rightarrow_{\tau}$ Computed $t^{\prime}$ if $t \rightarrow_{\tau} t^{\prime}$
12. Computed $t \rightarrow_{\tau} t$

Until now we have treated the Computed constructor just as the identity. We call an abstract machine term $t$ closed if checkfrees $0 t$ holds and for any subterm Computed s of $t$ the following assumptions hold:

- $s$ is a pure term, i.e. it does not contain Computed,
- checkfrees 0 s holds,
- there is no $s^{\prime}$ with $s \rightarrow_{\beta} s^{\prime}$.

Definition 2.11 - An abstract machine is a mapping that takes an abstract machine program to a Abstract Machine
relation $\rightarrow_{A M}$ on closed abstract machine terms such that $\rightarrow_{A M}$ is a partial function and such that $t \rightarrow_{A M} t^{\prime}$ implies

- $t \Rightarrow{ }_{\tau} t^{\prime}$,
- $t^{\prime}$ is a pure term,
- there is no $t^{\prime \prime}$ such that $t^{\prime} \rightarrow_{\beta} t^{\prime \prime}$.

Note that an abstract machine is allowed to always fail, i.e. to map every program to the empty relation. This particular abstract machine would not be very useful, but our focus is on ensuring that if an abstract machine does compute something, it will be correct. The definition of what constitutes an abstract machine is designed to fulfill this promise while at the same time preserving some freedom for the abstract machine implementor. So when computing a term $t$ an abstract machine can assume that $t$ contains no free variables, and that subterms of $t$ marked with Computed have no $\beta$ redexes left. It must ensure when returning a result $t^{\prime}$ that any computing done can be understood in terms of $\tau$ reduction, that $t^{\prime}$ contains no Computed markers any more, and that there are no $\beta$ redexes left in $t^{\prime}$.

### 2.5.2 The Barras Machine

The most general implementation of the abstract machine interface that the HCL provides is the Barras machine. It is an interpreter with an execution model that is borrowed from the machine in [2]. The most important difference between ours and the original one is that the original one actually produces proofs by operating
on theorems instead of terms. Because of this no proof of correctness is given in [2]; we will provide a proof of partial correctness which shows that the Barras machine is a correct implementation of the abstract machine interface. Another difference is that we also allow guards.

The Barras machine mimicks the evaluation strategy of strict functional programming languages. It performs bottom-up evaluation; $\beta$ reductions are delayed via explicit substitutions.

The data structure of Barras terms is the one for abstract machine terms augmented with an additional constructor Closure for performing explicit substitutions. The Computed constructor is inherited from the definition of abstract machine terms and does not appear in [2].

$$
\begin{aligned}
\text { term }::= & \operatorname{Var} v \mid \text { Const } c\left|\operatorname{term}_{1} \cdot \operatorname{term}_{2}\right| \lambda \text { term } \mid \text { Computed term } \\
& \mid \text { Closure }\left[\text { term }_{0}, \ldots, \text { term }_{n}\right] \text { term }
\end{aligned}
$$

Any abstract machine term is also a Barras term. On the other hand, any Barras term can be understood as an abstract machine term by viewing Closure as a function defined by

$$
\text { Closure }\left[s_{1}, \ldots, s_{n}\right] t:=(\underbrace{\lambda \ldots \lambda}_{n \text { times }} t) \cdot s_{n} \cdot \ldots \cdot s_{1}
$$

instead of viewing Closure as a constructor.
The idea of the Closure constructor is to delay actual $\beta$ reduction until all arguments of a function have been collected. An additional intuition is that in a term of the form Closure $E t$ the Closure constructor acts as a marker that $t$ has not been computed yet.

The state $(s, t)$ of the Barras machine consists of the subterm $t$ that is currently reduced and a stack $s$ that keeps track of the position of this subterm in the larger term under consideration.

```
stack ::= SEmpty | SAppL term stack | SAppR term stack | SAbs c stack
```

- Definition 2.13 Barras Stack
Let us denote the larger term that $(s, t)$ encodes with $(s, t)_{\text {zoom out }}$ :

| $(\text { SEmpty, } t)_{\text {zoom out }}$ | $=\mathrm{t}$ |
| :--- | :--- |
| $\left(\text { SAppL } t_{2} s, t_{1}\right)_{\text {zoom out }}$ | $=\left(s, t_{1} \cdot t_{2}\right)_{\text {zoom out }}$ |
| $\left(\text { SAppR } t_{1} s, t_{2}\right)_{\text {zoom out }}$ | $=\left(s, t_{1} \cdot t_{2}\right)_{\text {zoom out }}$ |
| $(\text { SAbsc } s, t)_{\text {zoom out }}$ | $=(s, \lambda(t[(\operatorname{Var} 0) /(\text { Const } c)]))_{\text {zoom out }}$ |

In the above we substitute a variable for a constant. Let us give a definition for this:

| $($ Const $d)[(\operatorname{Var} v) /($ Const $c)]$ | $= \begin{cases}\operatorname{Var} v & \text { if } c=d \\ \text { Const } \quad \text { if } c \neq d\end{cases}$ | Definition 2.14 <br> Substituting a |
| :--- | :--- | :--- |
| $(\operatorname{Var} w)[(\operatorname{Var} v) /(\operatorname{Const} c)]$ | $=$ | Var $w$ |$\quad$| Variable for a |
| :--- |

Definition 2.15
Weak Reduction

Definition 2.16
Strong Reduction

Definition 2.17 Simplification

The Barras machine performs both strong and weak reduction. Weak reduction will not reduce those terms $\lambda t$ which are not applied to an argument; with strong reduction, if $t$ reduces to $t^{\prime}$, then $\lambda t$ will reduce to $\lambda t^{\prime}$. Because functional programming languages only perform weak reduction, the Barras machine will only perform strong reduction when no further weak reduction is possible.

1. weak $\left(s, \operatorname{Closure} E\left(t_{1} \cdot t_{2}\right)\right)=$ weak $\left(\operatorname{SAppL}\left(\right.\right.$ Closure $\left.E t_{2}\right)$ s, Closure $\left.E t_{1}\right)$
2. weak (SAppL t' $s$, Closure $\left.\left[e_{1}, \ldots, e_{n}\right](\lambda t)\right)=$ weak $\left(s\right.$, Closure $\left.\left[t^{\prime}, e_{1}, \ldots, e_{n}\right] t\right)$
3. weak $\left(s\right.$, Closure $\left.\left[e_{0}, \ldots, e_{n}\right](\operatorname{Var} v)\right)=$ weak $\left(s, e_{v}\right)$
4. weak $(s$, Closure $E($ Const $c))=$ weak ( $s$, Const $c)$
5. weak (s, Closure E (Computed $t))= \begin{cases}\text { weak }(s, \text { Closure }[] t) & \text { if } t \text { contains any } \lambda \\ \text { weak }(s, t) & \text { otherwise }\end{cases}$
weak $(s, t)= \begin{cases}\text { weak }(s, r) & \text { if match } t=\text { Some } r \\ \text { weak }(s, t) & \text { if match } t=\text { None }\end{cases}$
weak' $\left(S A p p R t_{1} s, t_{2}\right)=$ weak $\left(s, t_{1} \cdot t_{2}\right)$
weak' $\left(S A p p L t_{2} s, t_{1}\right)=\operatorname{weak}\left(S A p p R t_{1} s, t_{2}\right)$
weak' $(s, t)=(s, t)$
The reduction rules should be read like an ML function definition, i.e. rule $i$ will only be applied if there is no applicable rule $j$ with $j<i$. Because of guards, strong and weak reduction are mutually recursive; above rules need a definition of the match operation to be complete, and match depends on strong reduction. Therefore we first describe strong reduction, and look only then at the match operation.
6. $\operatorname{strong}\left(s\right.$, Closure $\left.\left[e_{1}, \ldots, e_{n}\right](\lambda t)\right)=\operatorname{strong}\left(\right.$ SAbs c $\left.s, t^{\prime}\right)$
where a) $c \in \mathbb{Z}$ is some fresh identifier not referring to any constant in $e_{1}, \ldots, e_{n}$ or in $t$ or in the abstract machine program
b) weak (SEmpty, Closure [Const c, $\left.\left.e_{1}, \ldots, e_{n}\right] t\right)=\left(S E m p t y, t^{\prime}\right)$
strong $\left(s, t_{1} \cdot t_{2}\right)=\operatorname{strong}\left(S A p p L t_{2} s, t_{1}\right)$
strong $(s, t)=$ strong $^{\prime}(s, t)$
strong' $($ SAbs c $s, t)=$ strong' $^{\prime}(s, \lambda(t[(\operatorname{Var} 0) /($ Const $c)]))$
strong' $\left(S A p p L t_{2} s, t_{1}\right)=$ strong $\left(S A p p R t_{1} s, t_{2}\right)$
strong' $\left(S A p p R t_{1} s, t_{2}\right)=\operatorname{strong}^{\prime}\left(s, t_{1} \cdot t_{2}\right)$
strong ${ }^{\prime}(s, t)=(s, t)$
Let simp be the partial function defined by

$$
\operatorname{simp} t=t^{\prime} \quad \text { if } \quad \text { weak }(\text { SEmpty }, t)=\left(\text { SEmpty }, t^{\prime \prime}\right) \text { and strong }\left(\text { SEmpty }, t^{\prime \prime}\right)=\left(\text { SEmpty }, t^{\prime}\right) .
$$

Definition 2.18 Let the abstract machine rule Matching

$$
\left(\left[\left(a_{1}, b_{1}\right), \ldots,\left(a_{n}, b_{n}\right)\right], p, t\right)
$$

be the first rule of the abstract machine program such that

1. $[p]_{T}[\zeta]=m$ for some substitution $\zeta=\left(0 \mapsto e_{0}, \ldots,|p|-1 \mapsto e_{|p|-1}\right)$,
2. $E=\left[e_{0}, \ldots, e_{|p|-1}\right]$,
3. $\operatorname{simp}\left(\right.$ Closure $\left.E a_{i}\right)=\operatorname{simp}\left(\right.$ Closure $\left.E b_{i}\right)$ for all $i=1, \ldots, n$.

Then we define

$$
\text { match } m=\text { Some (Closure E } t \text { ), }
$$

otherwise match $m=$ None.

The Barras machine maps an abstract machine program to the relation $\rightarrow_{\text {Barras }}$ where

$$
t \rightarrow_{\text {Barras }} t^{\prime} \quad \text { if } \operatorname{simp}(\text { Closure }[] t)=t^{\prime}
$$

The Barras machine is an abstract machine in the sense of Definition 2.11.
Proof. The $\rightarrow_{\text {Barras }}$ relation is defined in terms of simp, therefore it is a partial function. Let us assume that $t_{0} \rightarrow_{\text {Barras }} t_{F}$ holds. Then the machine state (SEmpty, $t_{0}$ ) has been transformed into the state (SEmpty, $t_{F}$ ) via a series of calls to weak, weak', strong and strong'. Showing $t_{0} \Rightarrow_{\tau} t_{F}$ is equivalent to showing (SEmpty, $\left.t_{0}\right)_{\text {zoom out }} \Rightarrow_{\tau}$ (SEmpty, $\left.t_{F}\right)_{\text {zoom out }}$. Note that when talking about $\tau$ reduction of Barras terms we view them as abstract machine terms by erasing all closures as explained earlier. Because $\Rightarrow_{\tau}$ is transitive, $t_{0} \Rightarrow_{\tau} t_{F}$ follows if we can show $\left(s_{1}, t_{1}\right)_{\text {zoom out }} \Rightarrow_{\tau}$ $\left(s_{2}, t_{2}\right)_{\text {zoom out }}$ for all consecutive states of the transformation of (SEmpty, $t_{0}$ ) into (SEmpty, $t_{F}$ ). We can assume for any state $(s, t)$ participating in the transformation the following invariant:

- $t$ is closed (when viewed as an abstract machine term),
- any term appearing in the stack $s$ is closed,
- for any subterm $c$ of $t$ or any term appearing in the stack such that $c$ is of shape Closure $\left[e_{1}, \ldots, e_{n}\right] t^{\prime}$, we have that $c$ and all $e_{i}$ are closed,
- if SAbs c s' appears somewhere in $s$ then Const $c$ does not appear anywhere in the abstract machine program.

This invariant is true for our initial state (SEmpty, $t_{0}$ ) as there are no terms in SEmpty and $t_{0}$ is a closed abstract machine term; both weak and strong reduction preserve this invariant. This is proven simultaneously with the compatibility of weak and strong reduction with $\tau$ reduction, but we do not mention this explicitly.

Why do we need that last condition in our invariant? Because it ensures compatibility of $\tau$ reduction with zooming out. All the time we will want to deduce from $t \Rightarrow_{\tau} t^{\prime}$ that also $(s, t)_{\text {zoom out }} \Rightarrow_{\tau}\left(s, t^{\prime}\right)_{\text {zoom out }}$ holds. If $s=S A b s c s^{\prime}$, then this is equivalent to $\left(s^{\prime}, t[(\operatorname{Var} 0) /(\text { Const } c)]\right)_{\text {zoom out }} \Rightarrow_{\tau}\left(s^{\prime}, t^{\prime}[(\operatorname{Var} 0) /(\text { Const } c)]\right)_{\text {zoom out }}$. But does $t[(\operatorname{Var} 0) /($ Const $c)] \Rightarrow_{\tau} t^{\prime}[(\operatorname{Var} 0) /($ Const $c)]$ hold? Yes, because Const $c$ does not appear in the abstract machine program. That way, $t \Rightarrow_{\tau} t^{\prime}$ is not due to any special properties that Const $c$ has with respect to the program. By induction it is therefore easy to show that $\tau$ reduction is compatible with zooming out.

Let us now check that $\tau$ reduction is compatible with each weak reduction rule.

1. From the definition of zooming out we conclude $\left(\operatorname{SAppL}\left(\text { Closure } E t_{2}\right) s \text {, Closure } E t_{1}\right)_{\text {zoom out }}=\left(s,\left(\text { Closure } E t_{1}\right) \cdot\left(\text { Closure } E t_{2}\right)\right)_{\text {zoom out }}$. Thus the compatibility follows from (Closure $\left.E t_{1}\right) \cdot\left(\right.$ Closure $\left.E t_{2}\right) \Rightarrow_{\tau}$ Closure $E\left(t_{1} \cdot t_{2}\right)$.
2. $\left(\text { SAppL } t^{\prime} s, \text { Closure }\left[e_{1}, \ldots, e_{n}\right](\lambda t)\right)_{\text {zoom out }}=\left(s,\left(\text { Closure }\left[e_{1}, \ldots, e_{n}\right](\lambda t)\right) \cdot t^{\prime}\right)_{\text {zoom out }}$, therefore the compatibility of rule 2 is a consequence of

$$
\begin{aligned}
\left(\text { Closure }\left[e_{1}, \ldots, e_{n}\right](\lambda t)\right) \cdot t^{\prime} & =(\underbrace{(\lambda \ldots \lambda}_{n \text { times }}(\lambda t)) \cdot e_{n} \cdot \ldots \cdot e_{1}) \cdot t^{\prime} \\
& =\underbrace{(\lambda \ldots \lambda}_{(n+1) \text { times }} t) \cdot e_{n} \cdot \ldots \cdot e_{1} \cdot t^{\prime} \\
& =\text { Closure }\left[t^{\prime}, e_{1}, \ldots, e_{n}\right] t .
\end{aligned}
$$

4 Definition 2.19
Barras Machine

- Theorem 2.1

Partial Correctness of the Barras Machine
3. The invariant tells us that Closure $\left[e_{0}, \ldots, e_{n}\right]$ (Var $\left.v\right)$ is closed. Thus $v \leq n$ and

$$
\operatorname{Closure}\left[e_{0}, \ldots, e_{n}\right](\operatorname{Var} v)=(\lambda \ldots \lambda(\operatorname{Var} v)) \cdot e_{n} \cdot \ldots \cdot e_{0} \Rightarrow{ }_{\tau} \quad e_{v} .
$$

4. Similarly, Closure $E$ (Const $c$ ) $\Rightarrow_{\tau}$ Const c.
5. The invariant ensures that in Closure $E$ (Computed $t$ ) the term $t$ is closed. Therefore

$$
\text { Closure E (Computed } t) \quad \Rightarrow_{\tau} \quad \text { Closure } E t \quad \Rightarrow_{\tau} \quad t .
$$

6. If no rule matches then the transformation is just the identity and there is nothing to show. On the other hand, assume that the state $(s, t)$ is transformed into $(s, r)$ by matching with the rule $\left(\left[\left(a_{1}, b_{1}\right), \ldots,\left(a_{n}, b_{n}\right)\right], p, u\right)$. Then
(a) $[p]_{T}[\zeta]=t$ for some substitution $\zeta=\left(0 \mapsto e_{0}, \ldots,|p|-1 \mapsto e_{|p|-1}\right)$,
(b) $E=\left[e_{0}, \ldots, e_{|p|-1}\right]$,
(c) $\operatorname{simp}\left(\right.$ Closure $\left.E a_{i}\right)=\operatorname{simp}\left(\right.$ Closure $\left.E b_{i}\right)$ for all $i=1, \ldots, n$,
and $r=$ Closure $E u$.
Inductively, we derive Closure $E a_{i}={ }_{\tau}$ Closure $E b_{i}$ for all $i=1, \ldots, n$. Because $u$ and all $a_{i}$ and $b_{i}$ contain no free variables except those for which $\zeta$ is defined, we have $u[\zeta] \Rightarrow{ }_{\tau}$ Closure $E u$ and $a_{i}[\zeta] \Rightarrow{ }_{\tau}$ Closure $E a_{i}$ and $b_{i}[\zeta] \Rightarrow{ }_{\tau}$ Closure $E b_{i}$. Thus rule 2 of Definition 2.10 for $\tau$ reduction is applicable and gives us $t=[p]_{T}[\zeta] \rightarrow_{\tau} u[\zeta] \Rightarrow_{\tau} r$.
The compatibility of rules 7 and 8 follows directly from the definition of zooming out, for rule 9 there is nothing to show.

Next are the strong reduction rules.

1. $\left(\text { SAbs c s }, t^{\prime}\right)_{\text {zoom out }}=\left(s, \lambda t^{\prime}[(\operatorname{Var} 0) /(\text { Const } c)]\right)_{\text {zoom out }}$. The term $t^{\prime}$ is the result of weakly reducing Closure [Const $c, e_{1}, \ldots, e_{n}$ ] $t$ and thus by induction

$$
\text { Closure }\left[\text { Const } c, e_{1}, \ldots, e_{n}\right] t \quad \Rightarrow_{\tau} \quad t^{\prime}
$$

From there we deduce

$$
\left(\text { Closure }\left[\text { Const } c, e_{1}, \ldots, e_{n}\right] t\right)[(\operatorname{Var} 0) /(\text { Const } c)] \quad \Rightarrow_{\tau} \quad t^{\prime}[(\operatorname{Var} 0) /(\text { Const } c)]
$$

because Const $c$ does not appear anywhere in the abstract machine program. Furthermore, Const $c$ does not appear in $e_{1}, \ldots, e_{n}$ and neither in $t$. Thus

$$
\begin{aligned}
\lambda t^{\prime}[(\operatorname{Var} 0) /(\text { Const } c)] & \Leftarrow_{\tau} \lambda\left(\left(\text { Closure }\left[\text { Const } c, e_{1}, \ldots, e_{n}\right] t\right)[(\operatorname{Var} 0) /(\text { Const } c)]\right) \\
& =\lambda\left(\text { Closure }\left[\operatorname{Var} 0, e_{1}, \ldots, e_{n}\right] t\right) \\
& =\lambda((\underbrace{\lambda \ldots \lambda} t) \cdot e_{n} \cdot \ldots \cdot e_{1} \cdot \operatorname{Var} 0) \\
& =\lambda((\operatorname{los}) \text { times } \\
& \left.\left.=\lambda\left(e_{1}, \ldots, e_{n}\right](\lambda t)\right) \cdot \operatorname{Var} 0\right) \\
& \Leftarrow_{\tau} \quad \text { Closure }\left[e_{1}, \ldots, e_{n}\right](\lambda t) .
\end{aligned}
$$

4. Follows directly from the definition of zooming out.

Zooming out leads to immediate proofs for all other strong reduction rules.
Actually, we are not done yet with the proof. To complete the proof that the Barras machine is a true abstract machine, we also have to show that from $t_{0} \rightarrow_{\text {Barras }} t_{F}$ it follows that $t_{F}$ contains no $\beta$-redexes, no Computed terms, and no closures anymore.

Proof. For the purpose of this part of the proof, we do not freely interchange Barras terms and abstract machine terms any longer; this means that we view Closure as a constructor now, and not as an abbreviation for a special kind of abstract machine term.

We say that a Barras term $w$ is in weak normal form (WNF) if it meets all of the following conditions:

1. If $w$ contains $\lambda$ s then those are always contained in a surrounding closure.
2. $w$ contains no closures except those of shape Closure $E(\lambda t)$.
3. $w$ does not contain any term of shape (Closure $E(\lambda t)) \cdot s$.
4. If $w$ contains $\beta$-redexes then those are always contained in a surrounding closure.
5. If $w$ contains Computed terms then those are always contained in a surrounding closure.

We first look at weak reduction and prove by induction over the number of reduction steps that its execution preserves the following invariants of the state $(S, T)$ of the Barras machine:
(I1) If Closure $\left[e_{1}, \ldots, e_{n}\right] t$ is contained in $T$ or in any of the terms in the stack $S$, then each $e_{i}$ is a closure or a WNF, and $t$ contains no closures.
(I2) $T$ and all terms in $S$ are closures or WNFs.
(I3) If $S A p p L t s$ is contained in $S$ then $t$ is a closure.
(I4) If $S A p p R t s$ is contained in $S$ then $t$ is a WNF.
It is easy to see that all the rules of reduction for weak and weak' preserve these four invariants:

- Let us start with (I3). SAppL $t s$ is only produced in rule 1 , and $t$ is clearly a closure there.
- To show (I4), note that $S A p p R t s$ is only produced in rule 8 ; $t$ cannot be a closure because otherwise one of the rules 1 to 5 would have been called; because of (I1) these rules form a complete case distinction on closures (at least for an SAPpL stack). Because of (I2) it follows that $t$ is a WNF.
- It is time to approach (I1). The only critical rules are 2 and 6 . Rule 2 preserves (I1) because of (I3). Rule 6 uses the fact that if match $t$ succeeds then $t$ cannot be a closure and must therefore be a WNF because of (I2).
- Critical for (I2) are the rules 5 and 7. Rule 5 is defined via a case distinction just so that (I2) is evident. In rule 7 the term $t_{1} \cdot t_{2}$ is a WNF because $t_{1}$ is a WNF but no closure (because of (I4)) and because $t_{2}$ is also a WNF ( $t_{2}$ cannot be a closure and no WNF as otherwise one of the rules 1,3,4,5 had applied).

Provided the start state of weak reduction fulfills all four invariants it follows that the terminal state (SEmpty, $t$ ) fulfills the invariants. Therefore $t$ is a closure or a WNF. It cannot be a closure and not a WNF because then rule 9 would never have applied. Therefore $t$ is a WNF.

Now we look at strong reduction. We introduce two further normal forms. The weaker normal form (WRNF) is a still weaker form of the WNF which we obtain by not requiring property 1. A Barras term has strong normal form (SNF) if it does not contain any closures.

The invariants for the state $(S, T)$ during strong reduction are then:
(J1) If Closure $\left[e_{1}, \ldots, e_{n}\right] t$ is contained in $T$ or in any of the terms in the stack $S$, then each $e_{i}$ is a closure or a WNF, and $t$ contains no closures.
(J2) $(S, T)_{\text {zoom out }}$ is a WRNF.
(J3) In every call strong $(S, T), T$ is a WNF.
(J4) In every call strong' $(S, T), T$ is a SNF.
(J5) If $S A p p L t s$ is contained in $S$ then $t$ is a WNF.
(J6) If $S A p p R t s$ is contained in $S$ then $t$ is a SNF.
We want to prove that these invariants hold throughout strong reduction by induction over the number of strong and strong' reduction steps. As induction base, consider how strong reduction is called indirectly via $\operatorname{simp}$ (Closure [] $t$ ): first weak (SEmpty, Closure [] $t)=\left(\right.$ SEmpty, $\left.t^{\prime \prime}\right)$ leads to $t^{\prime \prime}$ and then strong (SEmpty, $t^{\prime \prime}$ ) is called. The state (SEmpty, Closure [] $t$ ) fulfills trivially all invariants I1 to I4 and therefore $t^{\prime \prime}$ is a WNF as we have proved before. This implies that all invariants J1 to J6 hold trivially for the call strong (SEmpty, $t^{\prime \prime}$ ).

The induction step is again easy to do; we just check that all the invariants stay true:

- Let us consider rule 1 of strong reduction. A call to

$$
\operatorname{strong}\left(s, \text { Closure }\left[e_{1}, \ldots, e_{n}\right](\lambda t)\right)
$$

results in a call to strong (SAbs c $s, t^{\prime}$ ) where $t^{\prime}$ is the result of

$$
\text { weak }\left(\text { SEmpty, Closure }\left[\text { Const } c, e_{1}, \ldots, e_{n}\right] t\right)=\left(\text { SEmpty, } t^{\prime}\right) .
$$

All invariants I1 to I4 are true for the state weak is called with: I1 holds because J 1 holds for ( $s$, Closure $\left[e_{1}, \ldots, e_{n}\right](\lambda t)$ ) and because Const $c$ is a WNF, similarly we derive I2 from J3. I3 and I4 hold trivially because the stack is empty.
Thus the result of weak reduction, $t^{\prime}$, is a WNF. Therefore J3 holds. There is no call to strong' which implies that J4 holds trivially. All closures appearing in $t^{\prime}$ have to respect I 1 and therefore also J1 holds. The stack SAbs $\mathrm{c} s$ inherits all $S A p p L$ and $S A p p R$ elements from $s$, therefore J5 and J6 hold trivially. The only invariant we have to be a little bit careful about is J2. In order for (SAbs c s, $\left.t^{\prime}\right)_{\text {zoom out }}$ to be a WRNF, we must ensure that it does not contain any $\beta$-redexes. Zooming one step out of (SAbscs, $t^{\prime}$ ) yields a state of the form ( $s, \lambda \ldots$ ), so there is the danger of introducing such a $\beta$-redex if s is an $S A p p L$ stack. Fortunately this cannot be the case, because otherwise property 3 of WRNF (we just use the same numbering of properties as for WNFs) would have been violated already in the original state.

- In rule 2 , we have that both $t_{1}$ and $t_{2}$ are WNFs because $t_{1} \cdot t_{2}$ is a WNF. Therefore J3 and J5 hold. The other invariants hold trivially.
- In rule 3 only invariant J4 needs special consideration. We have to show that $t$ is a SNF, i.e. $t$ contains no closures. We already assume because of J3 that $t$ must be a WNF. That means it cannot be a $\lambda$-term or a Computed term. It also cannot be an application, because otherwise rule 2 of strong reduction would
have applied instead of rule 3. It also cannot be a Closure: because $t$ is a WNF, it could only be a closure of shape Closure...( $\lambda \ldots$...), but closures of this shape would have been handled by rule 1 instead of rule 3 . Therefore $t$ must be a variable or a constant which both contain no closures. Therefore J4 holds.
- In rule 4 all invariants obviously hold.
- In rule 5, invariant J3 holds because of J5, and J6 because of J4.
- In rule 6, invariant J4 holds because of J4 and J6.
- In rule 7 all invariants obviously hold. Note that $s$ must be SEmpty and that rule 7 is always the last rule that is applied during strong reduction.

We have proven that all invariants J1 to J6 hold throughout strong reduction. Any terminal result (SEmpty, $t$ ) of strong reduction fulfills in particular J4 and J2. This implies that $t$ is both a SNF and a WRNF. Because it is a SNF, it contains no closures anymore. Because it is a WRNF, it does not contain any $\beta$-redexes or Computed terms anymore, because in a WRNF these constructs survive only within closures.

In Section 2.4.2 we described how to delay immediate evaluation of the last arguments of a function by moving them from the left hand side of a rule to the right hand side. This is directly supported by the Barras machine; actually, it is at the heart of its execution model. In order to evaluate Closure $E\left(t_{1} \cdot t_{2}\right), t_{2}$ is wrapped up in a closure and put into the stack in unevaluated form (weak reduction rule 1). Then Closure $E t_{1}$ is evaluated. The result of this evaluation might be an abstraction which does not reference its argument. In this case, $t_{2}$ will never be evaluated. One can summarize the evaluation strategy of the Barras machine as follows: $\beta$ reduction computes its argument lazily, application of a program rule computes all of the arguments strictly.

### 2.5.3 The SML Machine

The SML machine is currently the fastest implementation of the abstract machine interface. This is achieved by translating an abstract machine program directly to Standard ML code. The SML machine is not as general as the Barras machine; abstract machine terms of shape $\lambda t$ are translated to SML functions, which can only be applied, but not inspected for their body $t$. Therefore if the result of the computation still contains SML functions, it cannot be translated back to an abstract machine term. This restriction could be lifted by a more complex translation from $\lambda$ terms to SML functions which also wires some form of term management into the SML functions. But our experiments seem to indicate that this irrevocably leads to a severe degradation of computing performance by a factor of 5 to 10 . Therefore, in order to achieve maximal speed, the generality of the SML machine has been sacrificed. Note that this is not as big a restriction as it may sound:

- When compared to the Barras machine, this just means that the SML machine does not perform strong reduction but only weak reduction.
- Constants may represent functions; only the ability to return anonymous functions is lost.
- Anonymous functions can be used during the computation; only at the end they need to be gone.

An SML program basically consists of data structures and the functions that operate on them. Earlier we showed an example of how computing with numerals can be encoded in SML (fig. 2.8). The data structure there is a datatype made up of the four constructors Zero, Neg1, B0 and B1. The functions are those for addition add, multiplication mult and so on. We would like the SML machine to produce similar code for the abstract machine program consisting of the rules in Figures 2.4-2.7. There seems to be a straightforward enough recipe; divide all constants into two kinds, the function constants, and the data constants. The function constants are those constants which appear as head symbols on the left hand side of a program rule, e.g. neg, as it appears as a head symbol in the rule neg Zero = Zero. The data constants are those constants appearing in the rules which are not function constants, e.g. Zero. Then generate a datatype definition containing all data constants as constructors, and one function definition for each function constant.

This simple recipe would actually be an adequate one if we were generating SML code for Figures 2.4-2.6 only. But the rules in Figure 2.7 complicate things, because now both $B_{0}$ and $B_{1}$ are function constants and therefore no longer data constants. This cripples our datatype. There is also the problem of the norm function in Figure 2.8. Its origin is in the rules of Figure 2.7, obviously, but how exactly is the SML function norm derived from those rules?

Figuring out stuff like this is nothing an automatic translation tool is very good at. Fortunately, we can modify our simple recipe to get another simple recipe. Who says that the sets of function constants and data constants must be disjunct? We just change our definition of data constants: any constant appearing in the rules is a data constant. Therefore function constants are special data constants. This means that $B_{0}$ and $B_{1}$ both have two SML incarnations. They are translated into SML constructors BQ and B1. And they are translated into SML functions b0 and b1:

```
fun b0 Zero = Zero
    | b0 x = BO x
```

```
fun b1 Neg1 = Neg1
```

fun b1 Neg1 = Neg1
| b1 x = B1 x

```
    | b1 x = B1 x
```

The set $\mathcal{D} \subset \mathbb{Z}$ is the set of data constants, i.e. Const $c$ appears in any of the rules of the abstract machine program iff $c \in \mathcal{D}$.

The set $\mathcal{F} \subset \mathcal{D}$ is the set of function constants, i.e. $c \in \mathcal{F}$ iff there is a rule $r=$ ( $\left[g_{1}, \ldots, g_{n}\right], p, t$ ) of the abstract machine program and $p$ has shape PConstc $\left[p_{1}, \ldots, p_{m}\right]$. We say then that $r$ belongs to the function constant $c$.

We assume that the input of the SML machine consists not only of the abstract machine program but also of an arity function $\phi$. There is no restriction on $\phi$ except that it be a function from $\mathbb{Z}$ to $\mathbb{N}$. The arity $\phi$ is critical to the behavior of the SML machine. Nevertheless, the SML machine is required to implement the abstract machine interface, no matter what $\phi$ might be.

A pattern PConst c $\left[p_{1}, \ldots, p_{n}\right.$ ] is called compatible with the arity function $\phi$ if $\phi(c)=n$ holds and if all $p_{i}$ for $i=1, \ldots, m$ are compatible with $\phi$. We modify the given abstract machine program in the following way:

1. Any rule ( $\left[g_{1}, \ldots, g_{m}\right]$, PConst $\left.c\left[p_{1}, \ldots p_{n}\right], t\right)$ with $n>\phi(c)$ or any incompatible $p_{i}$ is removed.
2. Each rule $\left(\left[\left(a_{1}, b_{1}\right), \ldots,\left(a_{m}, b_{m}\right)\right]\right.$, PConst $\left.c\left[p_{1}, \ldots, p_{n}\right], t\right)$ such that all $p_{i}$ are compatible and $\delta=\phi(c)-n \geq 0$ is replaced by the rule
$(\left[\left(a_{1} \uparrow^{\delta-1}, b_{1} \uparrow^{\delta-1}\right), \ldots,\left(a_{m} \uparrow^{\delta-1}, b_{m} \uparrow^{\delta-1}\right)\right]$, PConst $c[p_{1}, \ldots, p_{n}, \underbrace{P \operatorname{Var}, \ldots, P \operatorname{Var}}_{\delta \text { times }}], \tilde{t})$
where $\left(\ldots\left(t \uparrow^{\delta-1} \cdot \operatorname{Var}(\delta-1)\right) \cdot \ldots \cdot \operatorname{Var} 0\right) \rightarrow_{\beta}^{*} \tilde{t}$ and there is no $t^{\prime}$ with $\tilde{t} \rightarrow_{\beta} t^{\prime} .{ }^{3}$ We define $\uparrow^{-1}$ to be just the identity operator.
We also say that $c$ has at most lazy index $\delta$, and at least strict index $n$.
Note that if $a \Rightarrow_{\tau} b$ with respect to the modified program then also $a \Rightarrow_{\tau} b$ with respect to the original program. We can therefore forget the original program and work with the modified program but still claim that the SML machine implements the abstract machine interface correctly with respect to the original program as long as it implements the interface correctly with respect to the modified one. From now on we assume that only compatible patterns occur in the abstract machine program. With every function constant $c \in \mathcal{F}$ we associate its lazy index lazy (c), which is the least $i$ such that $c$ has at most lazy index $i$, and its strict index strict $(c)$, which is the greatest $i$ such that $c$ has at least strict index $i$. Lazy and strict index of $c$ sum up to

$$
\phi(c)=\operatorname{strict}(c)+\operatorname{lazy}(c) .
$$

Let $\mathcal{D}=\left\{c_{1}, \ldots, c_{n}\right\}$ be the set of size $n$ of data constants. The induced SML data structure Term is then defined by

$$
\begin{aligned}
\text { datatype Term } & =\text { App of Term * Term } \\
& \mid \text { Abs of (Term -> Term) } \\
\mid & \text { Const of int } \\
& \Phi\left(c_{1}\right) \\
\vdots & \\
& \Phi\left(c_{n}\right)
\end{aligned}
$$

where

$$
\Phi(c)= \begin{cases}C c & \text { if } \phi(c)=0 \\ C c \text { of } \underbrace{\text { Term } \ldots \ldots * \text { Term }}_{\phi(c) \text { times }} & \text { if } \phi(c)>0\end{cases}
$$

Assume $\mathcal{D}=\{0,3,8\}$, and $\phi(0)=4, \phi(3)=0, \phi(8)=1$. Then

$$
\begin{aligned}
& \Phi(0)=C Q \text { of Term * Term * Term * Term } \\
& \Phi(3)=C 3 \\
& \Phi(8)=C 8 \text { of Term }
\end{aligned}
$$

This is the induced SML data structure:

$$
\begin{array}{ll}
\text { datatype Term } & =\text { App of Term * Term } \\
& \text { | Abs of (Term -> Term) } \\
& \text { | Const of int } \\
& \text { | CO of Term * Term * Term * Term } \\
& \text { C3 } \\
& \text { C8 of Term }
\end{array}
$$

The SML equality operator $=$ is not defined for values of type Term because in order to compare Abs $f$ with Abs $g$ one would have to compare the two functions $f$ and g. But in order to cope with guarded rules we need to be able to compare two values of type Term for equality. Of course, this comparison will only be approximate, i.e. it might return false for values that will behave identical in all situations.

```
Definition \(2.22 \rightarrow\) eq (App \((a 1, a 2))(A p p(b 1, b 2)) \quad=\) eq a1 b1 andalso eq a2 b2
Equality for Term
\begin{tabular}{rl} 
eq (Abs \(u\) ) (Abs v) & \\
eq (Const c1) (Const c2) & false \\
eq \(\left(C_{c_{1}}\left(u_{1}, \ldots, \mathrm{u}_{\phi\left(c_{1}\right)}\right)\right)\left(\mathrm{C}_{1}\left(\mathrm{v}_{1}, \ldots, \mathrm{v}_{\phi\left(c_{1}\right)}\right)\right)\) & \(=\) eq \(=\mathrm{c} \mathrm{u}_{1} \mathrm{v}_{1}\) andalso \(\ldots\) andalso eq \(\mathrm{u}_{\phi\left(c_{1}\right)} \mathrm{v}_{\phi\left(c_{1}\right)}\) \\
& \(\vdots\) \\
eq \(\left(C_{c_{n}}\left(\mathrm{u}_{1}, \ldots, \mathrm{u}_{\phi\left(c_{n}\right)}\right)\right)\left(\mathrm{C}_{c_{n}}\left(\mathrm{v}_{1}, \ldots, \mathrm{v}_{\phi\left(c_{n}\right)}\right)\right)\) & \(=\) eq \(\mathrm{u}_{1} \mathrm{v}_{1}\) andalso \(\ldots\) andalso eq \(\mathrm{u}_{\phi\left(c_{n}\right)} \mathrm{v}_{\phi\left(c_{n}\right)}\) \\
eq u v & \(=\) false
\end{tabular}
```

An abstract machine pattern $p$ can be translated into a piece of SML code $[p]_{\text {SML }}^{k}$. Like in the translation from $p$ to $[p]_{T}$ we number the free variables of the pattern from right to left starting with 0 .

Definition 2.23
Translation of Abstract
Machine Patterns to SML

$$
\begin{aligned}
& {[\text { PConst } c[]]_{\mathrm{SML}}^{k}} \\
& {\left[\text { PConst }\left[p_{1}, \ldots, p_{n}\right]\right]_{\mathrm{SML}}^{k}}
\end{aligned}=[c]_{\mathrm{SML}}^{k}(),[]_{\mathrm{SML}}^{k} q_{1} \ldots q_{n} .
$$

$$
[c]_{\mathrm{SML}}^{k} \quad= \begin{cases}c c & \text { if } k=0 \\ c c^{\prime} k & \text { if } k>0\end{cases}
$$

$$
[P \operatorname{Var}]_{\mathrm{SML}, i} \quad=\mathrm{x} i
$$

$$
[\text { PConst } c[]]_{\mathrm{SML}, i}=\mathrm{Cc}
$$

$$
\left[\text { PConst } c\left[p_{1}, \ldots, p_{n}\right]_{\mathrm{SML}, i}=\mathrm{C} c\left(q_{1}, \ldots, q_{n}\right)\right.
$$

$$
\text { for } n>0 \text { where } q_{j}=\left[p_{j}\right]_{\mathrm{SML}, I(j)} \text { and } I(j)=i+\sum_{k=j+1}^{n}\left|p_{k}\right|
$$

Here are several examples of the translation from patterns to SML code:
Example 2.2 - $[\text { PConst } 8[P \operatorname{Var}]]_{\mathrm{SML}}^{0} \quad=\mathrm{c} 8(\mathrm{p} 1$ as x 0$)$
$[\text { PConst } 8[P \operatorname{Var}]]_{\text {SML }}^{3}=\mathrm{c} 8{ }^{3} 3(\mathrm{p} 1$ as x 0$)$
[PConst 3[]$]_{\text {SML }}^{0}=\mathrm{c} 3()$
$[\text { PConst } 3[]]_{\text {SML }}^{6}=c 3{ }^{\prime} 6()$
$[\text { PConst } 0[P \text { Var, PConst } 3[], P \operatorname{Var}, \text { PConst } 0[P V a r, P C o n s t ~ 8[P V a r], P V a r, P V a r]]]_{\mathrm{SML}}^{13}=$ C0'13 ( p 1 as x 5 ) ( p 2 as C3) ( p 3 as x 4 ) ( p 4 as CQ ( $\mathrm{x} 3, C 8(\mathrm{x} 2), \mathrm{x} 1, \mathrm{x} 0)$ )

Also, any abstract machine term can be translated into a piece of SML code. For a more concise description of the translation we introduce a new constructor Call for abstract machine terms which can also be viewed as an abbreviation

$$
\text { Call } c\left[t_{1}, \ldots, t_{n}\right]:=\left(\ldots\left((\text { Const } c) \cdot t_{1}\right) \cdot \ldots \cdot t_{n}\right)
$$

Definition 2.24
Introducing Call

| 1. | Const $c \rightarrow_{\text {call intro }}$ Call $c[]$ | if | $c \in \mathcal{D}$ |
| :--- | :--- | :--- | :--- |
| 2. | $\left(\right.$ Call $\left.c\left[a_{1}, \ldots, a_{n}\right]\right) \cdot b \rightarrow_{\text {call intro }}$ Call $c\left[a_{1}, \ldots, a_{n}, b\right]$ | if | $n<\phi(c)$ |
| 3. | $\lambda t \rightarrow_{\text {call intro }} \lambda t^{\prime}$ | if | $t \rightarrow$ call intro $t^{\prime}$ |
| 4. | $t_{1} \cdot t_{2} \rightarrow_{\text {call intro }}^{\prime} t_{1}^{\prime} \cdot t_{2}$ | if | $t_{1} \rightarrow_{\text {call intro }} t_{1}^{\prime}$ |
| 5. $t_{1} \cdot t_{2} \rightarrow_{\text {call intro }} t_{1} \cdot t_{2}^{\prime}$ | if | $t_{2} \rightarrow_{\text {call intro }} t_{2}^{\prime}$ |  |
| 6. | Computed $t \rightarrow_{\text {call intro }}$ Computed $t^{\prime}$ | if | $t \rightarrow_{\text {call intro }} t^{\prime}$ |
| 7. | Call $c\left[\ldots, a_{i}, \ldots\right] \rightarrow_{\text {call intro }}$ Call $c\left[\ldots, a_{i}^{\prime}, \ldots\right]$ | if | $a_{i} \rightarrow_{\text {call intro }} a_{i}^{\prime}$ |

[^3]For our translation to always work and type check in SML, calls to function or data constants $c \in \mathcal{D}$ without supplying all of their arguments $\phi(c)$ must be prohibited. This can be achieved by performing $\eta$ abstraction where necessary.

1. Callc $\left[a_{1}, \ldots, a_{n}\right] \rightarrow_{\text {abstract }} \underbrace{\lambda \ldots \lambda}_{\delta \text { times }}\left(\operatorname{Call} c\left[a_{1} \uparrow^{\delta-1}, \ldots, a_{n} \uparrow^{\delta-1}, \operatorname{Var}(\delta-1), \ldots, \operatorname{Var} 0\right]\right)$

$$
\text { if } \quad \delta=\phi(c)-n>0
$$

2. $\lambda t \rightarrow_{\text {abstract }} \lambda t^{\prime} \quad$ if $t \rightarrow_{\text {abstract }} t^{\prime}$
3. $t_{1} \cdot t_{2} \rightarrow$ abstract $t_{1}^{\prime} \cdot t_{2} \quad$ if $t_{1} \rightarrow$ abstract $t_{1}^{\prime}$
4. $t_{1} \cdot t_{2} \rightarrow_{\text {abstract }} t_{1} \cdot t_{2}^{\prime} \quad$ if $t_{2} \rightarrow_{\text {abstract }} t_{2}^{\prime}$
5. Computed $t \rightarrow$ abstract Computed $t^{\prime}$ if $t \rightarrow_{\text {abstract }} t^{\prime}$
6. Call $c\left[\ldots, a_{i}, \ldots\right] \rightarrow_{\text {abstract }}$ Call $c\left[\ldots, a_{i}^{\prime}, \ldots\right] \quad$ if $\quad a_{i} \rightarrow_{\text {abstract }} a_{i}^{\prime}$

Given an abstract machine term $t$, let $[t]_{\text {call intro }}$ be the normal form with respect to $\rightarrow_{\text {call intro }}$, and $[t]_{\text {abstract }}$ the normal form with respect to $\rightarrow_{\text {abstract }}$. For the translation from an abstract machine term $t$ to its corresponding SML code $[t]_{\text {SML }}^{l}$ we reuse the notation that we have employed for the translation from patterns to SML code; note that the indices in the notation have a different meaning, though.

$$
\begin{aligned}
& {[t]_{\text {SML }}^{l} \quad=\left[\left[[t]_{\text {call intro }}\right]_{\text {abstract }}\right]_{\text {SML }, 0}^{l}} \\
& {[\text { Const c] }]_{\text {SML }, m}^{l}} \\
& =(\text { Const } c) \\
& {[\text { Var } v]_{\text {SML }, m}^{l}= \begin{cases}(\mathbf{b}(m-v-1)) & \text { if } v<m \\
(\mathrm{x}(v-m)()) & \text { if } m \leq v<m+l \\
(\mathrm{x}(v-m)) & \text { if } m+l \leq v\end{cases} } \\
& {[u \cdot v]_{\text {SML }, m}^{l} \quad=\left(\operatorname{app}[u]_{\text {SML }, m}^{l}[v]_{\text {SML }, m}^{l}\right)} \\
& \left.[\lambda t]_{\text {SML }, m}^{l} \quad=\text { (Abs (fn } \mathrm{b} m=[t]_{\mathrm{SML}, m+1}^{l}\right) \text { ) } \\
& {[\text { Computed } t]_{\mathrm{SML}, m}^{l}=[t]_{\mathrm{SML}, m}^{l}} \\
& {\left[\text { Call } c\left[t_{1}, \ldots, t_{n}\right]\right]_{\mathrm{SML}, m}^{l}= \begin{cases}\mathrm{C} c & \text { if } n=0 \text { and } c \notin \mathcal{F} \\
(\mathrm{Cc}(\mathrm{O}) & \text { if } n=0 \text { and } c \in \mathcal{F} \\
\left(\mathrm{C} c\left(\left[t_{1}\right]_{\mathrm{SML}, m}^{l}, \ldots,\left[t_{n}\right]_{\mathrm{SML}, m}^{l}\right)\right) & \text { if } n>0 \text { and } c \notin \mathcal{F}\end{cases} } \\
& {\left[\text { Call } c\left[t_{1}, \ldots, t_{n}\right]\right]_{\text {SML }, m}^{l}=} \\
& \text { (cc }\left[t_{1}\right]_{\text {SML }, m}^{l} \cdots\left[t_{\text {strict }(c)}\right]_{\text {SML }, m}^{l} \\
& \left.\left(\mathrm{fn}()=>\left[t_{\text {strict }(c)+1}\right]_{\text {SML }, m}^{l}\right) \ldots\left(\mathrm{fn}()=>\left[t_{\text {strict }(c)+\operatorname{lazy}(c)}\right]_{\text {SML }, m}^{l}\right)\right) \\
& \text { if } n>0 \text { and } c \in \mathcal{F}
\end{aligned}
$$

In the above we use the SML function app. Its definition is

```
fun app (Abs a) b = a b
    | app a b = App (a, b)
```

It is now time to deal with the question of how to translate the rules of the abstract machine program into SML functions. All rules which belong to the same function constant are grouped together. There are $|\mathcal{F}|$ such groups. Each group is converted to a bunch of mutual recursive SML functions. Actually, the generated SML functions of two different groups are also potentially mutually recursive. Therefore we specify for each abstract machine rule just an SML rule of the form $f p_{1} \ldots p_{n}=g$. The list of all such SML rules can then be converted into a list of mutual recursive SML function definitions by putting fun, $\mid$ or and as appropiate in front of each SML rule.

- Definition 2.25
$\eta$ Abstraction for Call
- Definition 2.26

Translation of Abstract Machine Terms to SML

Let $G_{c}=\left[r_{1}, \ldots, r_{n}\right]$ be the list of all rules of the abstract machine program which belong to the function constant $c \in \mathcal{F}$. With each $i \in\{1, \ldots, n+1\}$ we associate an index $k_{i}$ in the following way:

- We set $k_{1}=0$.
- For $i>1$ we set $k_{i}=k_{i-1}$ if $r_{i-1}$ has no guards, and $k_{i}=k_{i-1}+1$ otherwise.

The group $G_{c}$ is converted into $\left|\left\{k_{1}, \ldots, k_{n+1}\right\}\right|$ mutual recursive SML functions which together consist of $n+\left|\left\{k_{1}, \ldots, k_{n+1}\right\}\right|$ SML rules. Each rule

$$
r_{i}=\left(\left[\left(a_{1}, b_{1}\right), \ldots,\left(a_{m}, b_{m}\right)\right], p, t\right)
$$

is converted either for $m=0$ into the SML rule

$$
[p]_{\text {SML }}^{k_{i}}=[t]_{\text {SML }}^{\operatorname{lazy}(c)}
$$

or for $m>0$ into the SML rule

$$
\begin{aligned}
{[p]_{\text {SML }}^{k_{i}}=} & \text { if eq }\left[a_{1}\right]_{\text {SML }}^{\operatorname{lazy}(c)}\left[b_{1}\right]_{\text {SML }}^{\operatorname{lazy}(c)} \text { andalso } \ldots \text { andalso eq }\left[a_{m}\right]_{\text {SML }}^{\operatorname{lazy}(c)}\left[b_{m}\right]_{\text {SML }}^{\operatorname{lazy}(c)} \\
& \text { then }[t]_{\text {SML }}^{1 a z y(c)} \text { else }[c]_{\text {SML }}^{k_{n+1}} \mathrm{p}_{1} \ldots \mathrm{p}_{\phi(c)}
\end{aligned}
$$

This gives us $n$ SML rules for the function constant $c$.
For each $k \in\left\{k_{1}, \ldots, k_{n+1}\right\}$ we have a rule which is triggered when the SML function $[c]_{\text {SML }} k$ is applied to arguments for which there is no rule in the abstract machine program. For $\operatorname{strict}(c)=\phi(c)>0$ it is

$$
[c]_{\text {SML }}^{k} \mathrm{p}_{1} \ldots \mathrm{p}_{\phi(c)}=\mathrm{Cc}\left(\mathrm{p}_{1}, \ldots, \mathrm{p}_{\phi(c)}\right)
$$

For $\phi(c)=0$ the default rule is

$$
[c]_{\text {SML }}^{k}()=C c
$$

For lazy $(c)>0$ it is

$$
\left.[c]_{\text {SML }}^{k} \mathrm{p}_{1} \ldots \mathrm{p}_{\phi(c)}=\mathrm{Cc}\left(\mathrm{p}_{1}, \ldots, \mathrm{p}_{\text {strict }(c)}, \mathrm{p}_{\text {strict }(c)+1}(), \ldots, \mathrm{p}_{\text {strict }(c)+\operatorname{lazy}(c)}\right)\right)
$$

Actually, experience shows that this last case seems to be rather useless, because it evaluates all lazy arguments of a function and will therefore most likely lead to nontermination. When the default rule is triggered this normally indicates that the abstract machine program is missing additional rules for evaluating the strict arguments of the function. An alternative and more user-friendly default case for $\operatorname{lazy}(c)>0$ is

$$
[c]_{\text {SML }}^{k} \mathrm{p}_{1} \ldots \mathrm{p}_{\phi(c)}=\text { raise UnresolvedLazyCall }
$$

The semantics is usually the same, but in the second case the user will be informed of the failure of the SML machine not by nontermination, but by an exception.

We are almost there now. But before we can define the SML machine, we need to define how to convert an SML value $t$ of type Term back into an abstract machine term $[t]_{\text {AMT }}$. This is done in the obvious way:

Definition 2.27
Translation of SML Values of Type Term to Abstract Machine Terms

| $[\text { App }(a, b)]_{\text {AMT }}$ | $=[a]_{\text {AMT }} \cdot[b]_{\text {AMT }}$ |
| :--- | :--- |
| $[\text { Abs } a]_{\text {AMT }}$ | $=$ |
| $[$ undefined |  |
| $[\text { Const } c]_{\text {AMT }}$ | $=$ Constc |
| $\left[\begin{array}{cc}c & \left.\left(t_{1}, \ldots, t_{n}\right)\right]_{\text {AMT }}\end{array}\right.$ | $=\left(\ldots\left((\right.\right.$ Const $\left.\left.c) \cdot\left[t_{1}\right]_{\text {AMT }}\right) \cdot \ldots\right) \cdot\left[t_{n}\right]_{\text {AMT }}$ |

The translation is a partial function as it works only on SML values which do not contain Abs nodes.

Let $S$ be the SML program consisting of

- the Term data type definition given in Definition 2.21,
- the SML function eq defined in Definition 2.22,
- the SML function app defined in Equation 2.5,
- the mutual recursive SML functions made up of all the SML rules stemming from converting each group $G_{c}$ for all $c \in \mathcal{F}$.

The SML machine maps an arity function $\phi$ and an abstract machine program to the relation $\rightarrow_{\text {SML }}$ where

$$
t \rightarrow_{S M L} t^{\prime}
$$

if

1. $t$ is a closed abstract machine term,
2. the result of executing $[t]_{S M L}^{0}$ in the context of $S$ is the $S M L$ value $s$,
3. s does not contain any occurrences of Abs,
4. $t^{\prime}=[s]_{A M T}$.

Let us look at the power of a function. We can formalize this concept in Isabelle/HOL by defining a constant power which obeys the following equation:

$$
\begin{equation*}
\text { power } f n=\text { if test-le } n \text { then } \lambda x . x \text { else } \lambda x \text {. power } f\left(\text { add } n \operatorname{Neg}_{1}\right)(f x) \tag{2.6}
\end{equation*}
$$

Alternatively, we could use the following equation:

$$
\begin{equation*}
\text { power } f n x=\text { if test-le } n \text { then } x \text { else power } f\left(\operatorname{add} n \operatorname{Neg}_{1}\right)(f x) \tag{2.7}
\end{equation*}
$$

We could also describe power by the guarded equations

$$
\begin{align*}
\text { test-le } n & \equiv \text { True } \\
\text { test-le } n & \equiv \text { False } \tag{2.8}
\end{align*} \Rightarrow \text { power } f n x=x .
$$

Based on power we define the square of a nonnegative integer in terms of addition:
square $a=$ power (add $a) a$ Zero
This defines a function square such that square $a=a^{2}$ for $a \geq 0$. The abstract machine program for executing square consists of the following rules:

- those for add and add (fig. 2.5);
- those for normalizing numerals (fig. 2.7);
- those for test-le and test-less (fig. 2.9);
- those for If (eq. 2.4);
- those for power (either eq. 2.6 or eq. 2.7 or eq. 2.8);
- those for square (eq. 2.9).

The set of function constants is then

| $c$ | $c \in \mathcal{F}$ | $\phi(c)$ | strict $(c)$ | lazy $(c)$ |
| ---: | :---: | :---: | :---: | :---: |
| TRUE | no | 0 |  |  |
| FALSE | no | 0 |  |  |
| ZERO | no | 0 |  |  |
| NEG1 | no | 0 |  |  |
| B0 | yes | 1 | 1 | 0 |
| B1 | yes | 1 | 1 | 0 |
| ADD | yes | 2 | 2 | 0 |
| ADD1 | yes | 2 | 2 | 0 |
| TESTLE | yes | 1 | 1 | 0 |
| TESTLESS | yes | 1 | 1 | 0 |
| IF | yes | 3 | 1 | 2 |
|  |  |  | 2 | 1 |

Table 2.3: Arity, Strictness, Laziness for Elements of $\mathcal{D}$

$$
\mathcal{F}=\{B Q, B 1, \text { ADD }, ~ A D D 1, \text { TESTLE, TESTLESS, IF, POWER, SQUARE }\}
$$

and the set of data constants is $\mathcal{D}=\{$ TRUE, FALSE, ZERO, NEG1 $\} \cup \mathcal{F}$. For a more readable presentation, we use textual labels for the elements of $\mathcal{D}$. The assumed arity function $\phi$ and the derived functions lazy and strict are listed in Table 2.3. Note that lazy (POWER) and strict(POWER) depend on what choice we have made in selecting a rule for power from the three equations (2.6), (2.7) and (2.8). The resulting SML program $S$ is displayed in Figures 2.11, 2.12 and $2.13,2.14$ or 2.15 , respectively.

Let us compute $t=$ square $\left(B_{1}\left(B_{1}\right.\right.$ Zero $)$ ), which amounts to calculating $3^{2}$. Executing $[t]_{\text {SML }}^{0}=\mathrm{cSQUARE}(\mathrm{cB1}$ ( $\mathrm{cB1} 1$ CZERO) $)$ in the context of $S$ results in the SML value $s=\operatorname{CB1}$ (CBO (CBO (CB1 ZERO))). Translating $s$ back into the realm of abstract machine terms gives $[s]_{\text {AMT }}=B_{1}\left(B_{0}\left(B_{0}\left(B_{1}\right.\right.\right.$ Zero $\left.\left.)\right)\right)$, which is the numeral representation of 9 .

Let us also illustrate the restriction of the SML machine to fail on abstract machine terms which compute to terms still containing abstractions. Assuming we use choose Equation 2.7 or 2.8 as rule for power, translating $t=$ power (add Zero) Zero leads to

$$
[t]_{\text {SML }}^{0}=\operatorname{Abs}(f n \text { bo } \Rightarrow \text { cPOWER (Abs (fn b1 => cADD CZERO b1)) CZERO b0) }
$$

Executing $[t]_{\text {SML }}^{0}$ in the context of $S$ returns an SML value Abs $f$ for some $f$ of type Term -> Term. We do not have enough information to translate such an SML value back into an abstract machine term. On the other hand, executing $t=(\lambda x$.power (add Zero) Zero $x$ ) Zero is no problem:
app (Abs (fn b0 => cPOWER (Abs (fn b1 => cADD CZERO b1)) CZERO b0)) CZERO
computes to the SML value CZERO, and the corresponding abstract machine term is Zero.
Theorem 2.2 - The SML machine is for any arity function $\phi$ an abstract machine in the sense of Definition 2.11.

Proof. We do not provide a rigorous proof of this theorem. Such a proof would involve a semantics for SML, and then a proof that $\tau$ reduction on abstract machine terms corresponds to evaluation of the translations in SML. Let us rather just note

```
datatype Term =
        App of Term * Term
    | Abs of Term -> Term
    | Const of int
    | CTRUE | CFALSE | CZERO | CNEG1
    | CB0 of Term | CB1 of Term
    | CADD of Term * Term | CADD1 of Term * Term
    | CTESTLE of Term | CTESTLESS of Term
    | CIF of Term * Term * Term
    | CPOWER of Term * Term * Term
    | CSQUARE of Term
fun eq (App (a1, a2)) (App (b1, b2)) = eq a1 b1 andalso eq a2 b2
    | eq (Abs u) (Abs v) = false
    | eq (Const c1) (Const c2) = (c1 = c2)
    | eq CTRUE CTRUE = true
    | eq CFALSE CFALSE = true
    | eq CZERO CZERO = true
    | eq CNEG1 CNEG1 = true
    | eq (CBO u1) (CBO v1) = eq u1 v1
    | eq (CB1 u1) (CB1 v1) = eq u1 v1
    | eq (CADD (u1,u2)) (CADD (v1,v2)) = eq u1 v1 andalso eq u2 v2
    | eq (CADD1 (u1,u2)) (CADD1 (v1,v2)) = eq u1 v1 andalso eq u2 v2
    | eq (CTESTLE u1) (CTESTLE v1) = eq u1 v1
    | eq (CTESTLESS u1) (CTESTLESS v1) = eq u1 v1
    | eq (CIF (u1,u2,u3)) (CIF (v1,v2,v3)) = eq u1 v1 andalso eq u2 v2 andalso eq u3 v3
    | eq (CPOWER (u1,u2,u3)) (CPOWER (v1,v2,v3)) = eq u1 v1 andalso eq u2 v2 andalso eq u3 v3
    | eq (CSQUARE u1) (CSQUARE v1) = eq u1 v1
    | eq u v = false
fun app (Abs a) b = a b
    | app a b = App (a, b)
fun cBO CZERO = CZERO
    | cB0 p1 = CB0 p1
and cB1 (p1 as CNEG1) = CNEG1
    | cB1 p1 = CB1 p1
and cADD (p1 as (CB0 x1)) (p2 as (CBO x0)) = cB0 (cADD x1 x0)
    | cADD (p1 as (CBO x1)) (p2 as (CB1 x0)) = cB1 (cADD x1 x0)
    | CADD (p1 as (CB1 x1)) (p2 as (CB0 x0)) = cB1 (cADD x1 x0)
    | cADD (p1 as (CB1 x1)) (p2 as (CB1 x0)) = cB0 (cADD1 x1 x0)
    | cADD (p1 as CZERO) (p2 as x0) = x0
    | cADD (p1 as x0) (p2 as CZERO) = x0
    | cADD (p1 as CNEG1) (p2 as (CB0 x0)) = cB1 (cADD CNEG1 x0)
    | cADD (p1 as CNEG1) (p2 as (CB1 x0)) = cB0 x0
    | cADD (p1 as (CB0 x0)) (p2 as CNEG1) = cB1 (cADD x0 CNEG1)
    | cADD (p1 as (CB1 x0)) (p2 as CNEG1) = cBO x0
    | cADD (p1 as CNEG1) (p2 as CNEG1) = cBO CNEG1
    | cADD p1 p2 = CADD (p1, p2)
```

Figure 2.11: SML Program, Part 1

```
and cADD1 (p1 as (CBO x1)) (p2 as (CBO x0)) = cB1 (cADD x1 x0)
    | cADD1 (p1 as (CB0 x1)) (p2 as (CB1 x0)) = cB0 (cADD1 x1 x0)
    | cADD1 (p1 as (CB1 x1)) (p2 as (CBO x0)) = cB0 (cADD1 x1 x0)
    | cADD1 (p1 as (CB1 x1)) (p2 as (CB1 x0)) = cB1 (cADD1 x1 x0)
    | cADD1 (p1 as CNEG1) (p2 as x0) = x0
    | cADD1 (p1 as x0) (p2 as CNEG1) = x0
    | cADD1 (p1 as CZERO) (p2 as (CBO x0)) = cB1 x0
    | cADD1 (p1 as CZERO) (p2 as (CB1 x0)) = cB0 (cADD1 CZERO x0)
    | cADD1 (p1 as (CBO x0)) (p2 as CZERO) = cB1 x0
    | cADD1 (p1 as (CB1 x0)) (p2 as CZERO) = cB0 (cADD1 x0 CZERO)
    | cADD1 (p1 as CZERO) (p2 as CZERO) = cB1 CZERO
    | cADD1 p1 p2 = CADD1 (p1, p2)
and cTESTLE (p1 as CZERO) = CTRUE
    | cTESTLE (p1 as CNEG1) = CTRUE
    | cTESTLE (p1 as (CB0 x0)) = cTESTLE x0
    | cTESTLE (p1 as (CB1 x0)) = cTESTLESS x0
    | cTESTLE p1 = CTESTLE p1
and cTESTLESS (p1 as CZERO) = CFALSE
    | cTESTLESS (p1 as CNEG1) = CTRUE
    | cTESTLESS (p1 as (CBO x0)) = cTESTLESS x0
    | cTESTLESS (p1 as (CB1 x0)) = cTESTLESS x0
    | cTESTLESS p1 = CTESTLESS p1
and cIF (p1 as CTRUE) (p2 as x1) (p3 as x0) = x1 ()
    | cIF (p1 as CFALSE) (p2 as x1) (p3 as x0) = x0 ()
    | cIF p1 p2 p3 = raise UnresolvedLazyCall
```

Figure 2.12: SML Program, Part 2

```
and cPOWER (p1 as x2) (p2 as x1) (p3 as x0) =
        app (cIF (cTESTLE x1)
                (fn () => Abs (fn b0 => b0))
                    (fn () => Abs (fn b0 => cPOWER x2 (cADD x1 CNEG1) (fn () => app x2 bQ))))
            (x0 ())
    | cPOWER p1 p2 p3 = raise UnresolvedLazyCall
and cSQUARE (p1 as x0) = cPOWER (Abs (fn b0 => cADD x0 b0)) x0 (fn () => CZERO)
    | cSQUARE p1 = CSQUARE p1
```

Figure 2.13: SML Program, Part 3a (resulting from Equation 2.6)
and CPOWER ( p 1 as x 2 ) ( p 2 as x 1 ) ( p 3 as x 0 ) $=$
cIF (cTESTLE $x 1$ ) (fn () => x0) (fn () => cPOWER x2 (cADD x1 CNEG1) (app x2 x0))
| CPOWER p1 p2 p3 = CPOWER (p1, p2, p3)
and cSQUARE (p1 as x 0 ) = cPOWER (Abs ( $\mathrm{fn} \mathrm{bO}=>$ cADD x 0 bO ) ) x 0 CZERO
| cSQUARE p1 = CSQUARE p1

Figure 2.14: SML Program, Part 3b (resulting from Equation 2.7)

```
and cPOWER (p1 as x2) (p2 as x1) (p3 as x0) =
        if eq (cTESTLE x1) CTRUE then x0
        else CPOWER'1 p1 p2 p3
    | cPOWER p1 p2 p3 = CPOWER (p1, p2, p3)
and CPOWER'1 (p1 as x2) (p2 as x1) (p3 as x0) =
            if eq (cTESTLE x1) CFALSE then cPOWER x2 (cADD x1 CNEG1) (app x2 x0)
            else CPOWER'2 p1 p2 p3
    | CPOWER'1 p1 p2 p3 = CPOWER (p1, p2, p3)
and CPOWER'2 p1 p2 p3 = CPOWER (p1, p2, p3)
and cSQUARE (p1 as x0) = cPOWER (Abs (fn b0 => cADD x0 b0)) x0 CZERO
    | cSQUARE p1 = CSQUARE p1
```

Figure 2.15: SML Program, Part 3c (resulting from Equation 2.8)
that we use SML as a purely functional language without side effects. Moving from the left hand side of a generated SML function definition to the right hand side of it and evaluating then this right hand side can clearly be understood as $\tau$ reduction. Also, all massaging of abstract machine terms and patterns we perform when ensuring that the abstract machine program is compatible with $\phi$, and when translating $t$ to $[t]_{\mathrm{SML}}^{l}$, can also be understood in terms of $\tau$ reduction.

### 2.5.4 The Haskell Machine

The Haskell machine is just a simpler version of the SML machine. Because Haskell is a lazy language, there is no need to distinguish between lazy and strict arguments of a function; we can just treat all function arguments like we treated the strict function arguments. Apart from that we could just copy everything said in the previous subsection about the SML machine to this subsection with minor modifications due to the syntactic differences between Haskell and SML. If we were willing to invest a little more work, we could further simplify the translation from abstract machine terms to Haskell code by utilizing that Haskell already has a built-in concept of guards, and that Haskell allows functions of arity 0 .

### 2.6 The HCL Cokernel

The HCL cokernel provides secure access to the modes of the HCL. It can be understood as an additional kernel sitting beside the Isabelle kernel and we will discuss its facilities for producing theorems. We argue that the cokernel cannot produce any theorem that the Isabelle kernel could not also produce on its own. This is what it means for the cokernel to be secure.

### 2.6.1 A Bird's-Eye View of the Isabelle Kernel

The Isabelle kernel is built around the following main notions: types, terms, theorems and theories.

A theory $\mathfrak{I}$ can be viewed as a state of the kernel. This state has (among others) the following components:

- A set of axiomatic type classes, like ring or order.
- A set of type constructors, like real or prop or $\rightarrow$. Each type constructor has an associated arity. E.g. real and prop have both arity 0 , and $\rightarrow$ has arity 2 . The type constructors prop and $\rightarrow$ are part of every Isabelle theory.

A sort is a subset of the set of axiomatic type classes. Types are given via

$$
\text { type }::=T \operatorname{Var} \alpha S \mid T A p p ~ c\left(\text { type }_{1}, \ldots, \text { type }_{n}\right)
$$

where $\alpha$ is some identifier, $S$ is a sort, and $c$ is a type constructor with associated arity $n$. Instead of TApp $\rightarrow\left(\tau_{1}, \tau_{2}\right)$ we also write $\tau_{1} \rightarrow \tau_{2}$. Instead of TApp $c$ where $c$ has arity 0 we just write $c$. We call TVar $\alpha S$ type variable and often write $\alpha:: S$ for it. We call a type $\tau$ a ground type if it does not contain any type variable. We define the functional arity of a type $\tau$ to be 0 if $\tau$ is a type variable or not of shape $\tau_{1} \rightarrow \tau_{2}$, and to be $1+$ the functional arity of $\tau_{2}$ if it has shape $\tau_{1} \rightarrow \tau_{2}$.

There are two more components of the theory $\mathfrak{I}$ :

- A transitive instance relation $\leq$ on types such that $\tau_{1} \leq \tau_{2}$ if $\tau_{1}$ can be obtained from $\tau_{2}$ by instantiating type variables $T \operatorname{Var} \alpha S$. For example, in many theories we will have real $\leq \alpha::\{$ ring $\}$ and real $\rightarrow$ nat $\leq \alpha::\{$ ring $\} \rightarrow \beta::\{$ order $\}$, but not nat $\leq \alpha::\{r i n g\}$. As always, when instantiating a type variable it must be instantiated everywhere in the type, therefore we can never have real $\rightarrow \alpha::$ $\{$ ring $\} \leq \alpha::\{$ ring $\} \rightarrow \alpha::\{$ ring $\}$. We have ${ }^{4} \tau \leq \alpha::\{ \}$ for any type $\tau$. We just write $\alpha$ for $\alpha::\{ \}$.
- A set of constants. Each constant is associated with its most general type $\tau$. Equality $\equiv$ with most general type $\alpha \rightarrow \alpha \rightarrow$ prop and implication $\Longrightarrow$ with most general type prop $\rightarrow$ prop are both constants that are part of every Isabelle theory.

Isabelle terms use de-Bruijn indices [6] for local variables and names for free variables. There are two kinds of free variables, Free and Var.

| term | $:=$ | App term term $_{2}$ |
| ---: | :--- | :--- |
|  | Const c type |  |
|  | Var x type |  |
|  | Free $x$ type |  |
|  | $\lambda$ type. term |  |
|  | Bound $i$ |  |

In the above $c$ is a constant of the theory, $x$ is an identifier, and $i$ is a de-Bruijn index. We call a term welltyped if it can be assigned a type using the following typing rules:

Definition 2.29
Type of a Term

```
type(t)=\tau
type }\mp@subsup{0}{0}{}E(\mathrm{ Const c }\tau)=
type }\mp@subsup{0}{0}{}E(App\mp@subsup{t}{1}{}\mp@subsup{t}{2}{})=
type }E(\operatorname{Var}x\tau)=
type }E(\mathrm{ Free }x\tau)=
type }[\mp@subsup{\tau}{1}{},\ldots,\mp@subsup{\tau}{n}{}](\lambda\tau.t)=\tau->\mp@subsup{\tau}{}{\prime}\quad\mathrm{ if type }0[\tau,\mp@subsup{\tau}{1}{},\ldots,\mp@subsup{\tau}{n}{}]t=\mp@subsup{\tau}{}{\prime
```



[^4]When writing down terms we often use abbreviations whose meaning we take for obvious. For example, we will write $t_{1} \equiv t_{2}$ instead of

$$
\operatorname{App}\left(\operatorname{App}\left(\text { Const } \equiv\left(\text { type }\left(t_{1}\right) \rightarrow \operatorname{type}\left(t_{2}\right)\right)\right) t_{1}\right) t_{2}
$$

A theorem consists of the following components:

- Its proposition, which is a welltyped term of type prop.
- A set of hypotheses. A hypothesis is a welltyped term of type prop which does not contain any occurrences of Var.
- A set of sort hypotheses. A sort hypothesis is just a sort $S$. Its meaning is that it is assumed that there is a ground type $\tau$ such that $\tau \leq \alpha:: S$.

We write $t=(\mathcal{S}, \mathcal{H}, p)$ for a theorem $t$ with sort hypotheses $\mathcal{S}$, hypotheses $\mathcal{H}$ and proposition $p$. While the Isabelle kernel allows to access the components of a theorem, one cannot construct a theorem by giving its components. Theorems can only be constructed through a set of operations the kernel provides. Here are a few of those operations:

Reflexivity Given a welltyped term $t$, the kernel can construct the theorem ( $\mathcal{S},\{ \}, t \equiv$ $t$ ), where $\mathcal{S}$ is the set of all sorts occurring in $t$.

Transitivity of Equality Given two theorems $\left(\mathcal{S}_{1}, \mathcal{H}_{1}, t_{1} \equiv t_{2}\right)$ and $\left(\mathcal{S}_{2}, \mathcal{H}_{2}, t_{2} \equiv t_{3}\right)$, the kernel can construct the theorem $\left(\mathcal{S}_{1} \cup \mathcal{S}_{2}, \mathcal{H}_{1} \cup \mathcal{H}_{2}, t_{1} \equiv t_{3}\right)$.

Discarding Sort Hypotheses Given a ground type $\tau$, and a type variable $\alpha:: S$ such that $\tau \leq \alpha:: S$, and a theorem $(\mathcal{S}, \mathcal{H}, p)$, the kernel can construct the theorem $(\mathcal{S}-\{S\}, \mathcal{H}, p)$.

Instantiation of Type Variables Given different type variables $\alpha_{1}:: S_{1}, \ldots, \alpha_{n}:: S_{n}$, and $n$ types $\tau_{i}$ with $\tau_{i} \leq \alpha_{i}:: S_{i}$, and a theorem $(\mathcal{S}, \mathcal{H}, p)$, the kernel can construct the theorem $\left(\mathcal{S}, \mathcal{H}^{\prime}, p^{\prime}\right)$, where $\mathcal{H}^{\prime}$ originates from $\mathcal{H}$ and $p^{\prime}$ originates from $p$ by simultaneously replacing all occurrences of $\alpha_{i}:: S_{i}$ by $\tau_{i}$.

Instantiation of Variables Given different variables TFree $x_{1} \tau_{1}, \ldots$, TFree $x_{n} \tau_{n}$ and $n$ terms $t_{i}$ with type $\left(t_{i}\right)=\tau_{i}$, and a theorem $(\mathcal{S}, \mathcal{H}, p)$, the kernel can construct the theorem $\left(\mathcal{S}, \mathcal{H}^{\prime}, p^{\prime}\right)$, where $\mathcal{H}^{\prime}$ originates from $\mathcal{H}$ and $p^{\prime}$ originates from $p$ by simultaneously substituting (this may involve de-Bruijn lifting of the $t_{i}$ ) all occurrences of TFree $x_{i} \tau_{i}$ by $t_{i}$. The same is true when we use in the above TVar instead of TFree.
$\beta \eta$ reduction Given a welltyped term $t$, and another welltyped term $t^{\prime}$ such that $t^{\prime}$ results from $t$ by $\beta \eta$ reduction, the kernel can construct the theorem $(\mathcal{S},\{ \}, t \equiv$ $t^{\prime}$ ), where $\mathcal{S}$ is the set of all sorts occurring in $t$.

Modus Ponens Given two theorems $\left(\mathcal{S}_{1}, \mathcal{H}_{1}, a \Longrightarrow b\right)$ and $\left(\mathcal{S}_{2}, \mathcal{H}_{2}, a\right)$, the kernel can construct the theorem $\left(\mathcal{S}_{1} \cup \mathcal{S}_{2}, \mathcal{H}_{1} \cup \mathcal{H}_{2}, b\right)$.

### 2.6.2 Removing and Attaching Types

One of the reasons why computing using the Isabelle kernel is slow is that the basic datastructure for computing used by the Isabelle kernel is that of a theorem, which is made up of terms, which are stuffed with types not really needed for computing. These types must be manipulated during computation, and can grow awfully large. To avoid this performance pitfall, abstract machines compute on untyped terms. Therefore, in order to use any abstract machine for computation we need to bridge the gap between Isabelle terms, which are typed, and abstract machine terms.

So, how can we get rid of the types in Isabelle terms? Just dropping them like in going from Const $c \tau$ to Const $c$ is not an option. E.g., Isabelle allows the overloading of constants [34,27]. An example where overloading comes in handy is when looking at integers int and nonnegative integers nat. The constants for subtraction - and zero 0 can be used with both types. But the equations that these constants fulfill differ wildly. If 0 and 1 have type nat, then in Isabelle/HOL the equation $0-1=0$ holds. Applying this rewriting rule to $0-1$, where 0 and 1 have type int, is clearly desastrous.

There is an easy way out of these complications. The terms Const 0 int and Const 0 nat are different, so we map them to different abstract machine terms. The term Const 0 int could be mapped to Const 14, for example, and the term Const 0 nat to Const 15.

Definition 2.30 - We call an Isabelle term an atom if it is either a constant Const $c \tau$ or a variable Atoms Free $x \tau$ or Var $x \tau$. For an arbitrary Isabelle term $t$ we denote by atoms $(t)$ the set of all atoms occurring in $t$.

Definition 2.31 - An encoding $\sigma$ is a partial injective mapping from the set of all welltyped atoms of a Encoding theory to $\mathbb{Z}$. Any encoding $\sigma$ induces a total mapping $\bar{\sigma}$ from the set of all welltyped Isabelle terms $t$ with atoms $(t) \subseteq \operatorname{dom} \sigma$ to the set of closed pure abstract machine terms:

| $\bar{\sigma}($ Const $c \tau)$ | $=\operatorname{Const}(\sigma($ Const $c \tau))$ |
| :--- | :--- |
| $\bar{\sigma}(\operatorname{Var} x \tau)$ | $=\operatorname{Const}(\sigma(\operatorname{Var} x \tau))$ |
| $\bar{\sigma}($ Free $x \tau)$ | $=\operatorname{Const}(\sigma($ Free $x \tau))$ |
| $\bar{\sigma}($ App $u v)$ | $=(\bar{\sigma} u) \cdot(\bar{\sigma} v)$ |
| $\bar{\sigma}(\lambda \tau . t)$ | $=\lambda(\bar{\sigma} t)$ |
| $\bar{\sigma}($ Bound $i)$ | $=\operatorname{Var} i$ |

Let us assume now that we have an Isabelle term $t$ we would like to compute. Given an encoding $\sigma$ such that $t$ is in the domain of $\bar{\sigma}$, we convert $t$ to the abstract machine term $s=\bar{\sigma} t$. Computing $s$ with an abstract machine AM results in another abstract machine term $s^{\prime}$ with $s \rightarrow_{\mathrm{AM}} s^{\prime}$. Therefore the result of computing $t$ is $t^{\prime}=\bar{\sigma}^{-1} s^{\prime}$.

There is a flaw in this approach. The problem is that although $\sigma$ is an injective mapping, $\bar{\sigma}$ is not. This can be seen quickly:

$$
\bar{\sigma}(\lambda \text { int. Bound } 0)=\lambda(\operatorname{Var} 0)=\bar{\sigma}(\lambda \text { prop. Bound } 0) .
$$

Fortunately, we know more about $t^{\prime}$ than just $\bar{\sigma} t^{\prime}=s^{\prime}$. We also know that any $t^{\prime}$ acceptable to us must have the property type $(t)=$ type $\left(t^{\prime}\right)$. This is enough to find $t^{\prime}$.

Theorem $2.3 \vee \quad$ For any encoding $\sigma$, the mapping $t \mapsto(\bar{\sigma} t$, type $(t))$ is injective on the set of those
Reversibility of Encoding

Proof. Let us first note that if $t$ contains no $\beta$ redexes, then neither does $\bar{\sigma} t$. Thus we can prove the theorem by defining a function attach which for a type $\tau$ and a closed pure abstract machine term $s$ without $\beta$ redexes either returns the unique $t$ with type $(t)=\tau$ and $\bar{\sigma} t=s$ or signals failure if there is no such $t$. That $t$ must be unique will be clear from the function definition itself because for each case of the function definition there is no degree of freedom what result could be returned.

$$
\left.\begin{array}{ll}
\text { attach } \tau E(\text { Const } c) & = \begin{cases}\sigma^{-1} c & \text { if } c \in \operatorname{dom} \sigma \wedge \operatorname{type}\left(\sigma^{-1} c\right)=\tau \\
\text { failure } & \text { otherwise }\end{cases} \\
\text { attach } \tau E(\text { Var } i) & =\begin{array}{ll}
\text { Bound } i
\end{array} \\
\text { attach } \tau\left[\tau_{1}, \ldots, \tau_{n}\right](\lambda t) & = \begin{cases}\lambda \tau^{\prime} . \text { attach } \tau^{\prime \prime}\left[\tau^{\prime}, \tau_{1}, \ldots, \tau_{n}\right] t & \text { if } \tau=\tau^{\prime} \rightarrow \tau^{\prime \prime} \\
\text { failure }\end{cases} \\
\text { otherwise }
\end{array}\right\} \begin{aligned}
& \text { attach } \tau E\left(f \cdot u_{1} \cdot \ldots \cdot u_{n}\right) \\
&= \begin{cases}\text { App } \ldots\left(\text { App g } v_{1}\right) \ldots v_{n} & \text { if attach } E f=\left(g, \tau_{1} \rightarrow \ldots \rightarrow \tau_{n} \rightarrow \tau\right) \text { and } v_{i}=\text { attach } \tau_{i} E u_{i} \\
\text { otherwise }\end{cases} \\
& \text { attach }_{0} E(\text { Const } c)= \begin{cases}\left(\sigma^{-1} c, \text { type }\left(\sigma^{-1} c\right)\right) & \text { if } c \in \operatorname{dom} \sigma \\
\text { failure } & \text { otherwise }\end{cases} \\
& \text { attach }_{0}\left[\tau_{1}, \ldots, \tau_{n}\right](\text { Var } i)= \\
&\text { (Bound } \left.i, \tau_{i+1}\right)
\end{aligned}
$$

Note that when defining attach for a chain of applications $f \cdot u_{1} \cdot \ldots \cdot u_{n}$ we know that $f$ cannot be an application $f=f_{0} \cdot u_{0}$ because otherwise we would instead be looking at $f_{0}$ in the chain of applications $f_{0} \cdot u_{0} \cdot u_{1} \cdot \ldots \cdot u_{n}$. Also, $f$ cannot be an abstraction $\lambda t$ because then we would have found a $\beta$ redex. Therefore $f$ must either be a constant or a variable, and both of these cases are covered in the definition of attach ${ }_{0}$.

### 2.6.3 Computing Equations

A state of the Isabelle kernel is called a theory. The corresponding concept for the HCL cokernel is that of a computer. A computer contains all the information necessary for computing an Isabelle term. Given a computer $\mathfrak{C}$, and a welltyped Isabelle term $t$, the cokernel will compute $t$ to $t^{\prime}$ and upon success return the equation $t \equiv t^{\prime}$ as a theorem.

We create a computer $\mathfrak{C}$ by handing over to the cokernel the following items:

1. A theory $\mathfrak{I}$.
2. A mode $A M$, i.e. a tag $A M \in\{B A R R A S, S M L, H A S K E L L\}$ which indicates which abstract machine should be used for computing.
3. A list $\left[\Psi_{1}, \ldots, \Psi_{n}\right]$ of theorems of the theory $\mathfrak{I}$. The proposition $p_{i}$ of each theorem

$$
\Psi_{i}=\left(\mathcal{S}_{i}, \mathcal{H}_{i}, p_{i}\right)
$$

has the shape given in Equation 2.2.
The created computer $\mathfrak{C}=\left(\mathfrak{I}, \mathrm{AM}, \mathcal{S}, \mathcal{H}, \sigma, \rightarrow_{\mathrm{AM}}\right)$ consists of these components:

- The theory $\mathfrak{I}$ and the mode AM.
- The cummulative set of sort hypotheses $\mathcal{S}=\mathcal{S}_{1} \cup \ldots \cup \mathcal{S}_{n} \cup \mathcal{P}$ where $\mathcal{P}$ is the set of all sorts occurring in any of the $p_{i}$.
- The cummulative set of of hypotheses $\mathcal{H}=\mathcal{H}_{1} \cup \ldots \cup \mathcal{H}_{n}$.
- An encoding $\sigma$ induced by the set of propositions $\left\{p_{1}, \ldots, p_{n}\right\}$. Any encoding with atoms $\left(p_{i}\right) \subseteq \operatorname{dom} \sigma$ for all $i=1, \ldots, n$ will do.
- The partial abstract machine function $\rightarrow_{\mathrm{Am}}$ induced by the arity function $\phi$ and the abstract machine program $\left[r_{1}, \ldots, r_{n}\right]$.
There are several sensible choices for $\phi$. One is to define $\phi(d)$ as the functional arity of type $\left(\sigma^{-1} d\right)$. Another one is to inspect the abstract machine program and make a heuristic choice which is our current approach.
The abstract machine rule $r_{i}$ is derived from the proposition $p_{i}$ in the obvious way using the encoding $\sigma$. Note that we convert only Vars to pattern variables, but not Frees. Also converting Frees to pattern variables could lead to inconsistency as Frees may appear in the hypotheses $\mathcal{H}_{i}$, which is not the case for Vars.

The cokernel applies the computer $\mathfrak{C}$ to compute a welltyped term $t$ of the theory $\mathcal{T}$ in the following way: ${ }^{5}$

1. Calculate $s=\bar{\sigma} t$.
2. Calculate $s^{\prime}$ such that $s \rightarrow_{\mathrm{AM}} s^{\prime}$.
3. Upon successfully calculating $s^{\prime}$, calculate $t^{\prime}=\operatorname{attach}($ type $(t))[] s^{\prime}$.
4. Upon successfully calculating $t^{\prime}$, return the theorem $\Psi=\left(\mathcal{S} \cup \mathcal{S}_{t}, \mathcal{H}, t \equiv t^{\prime}\right)$, where $\mathcal{S}_{t}$ is the set of sorts occurring in $t$.

In order to show that the HCL cokernel is secure, we need to show that the theorem $\Psi$ could also have been proven using only the operations the Isabelle kernel provides. We know that

$$
\bar{\sigma} t \quad \Rightarrow_{\tau} \quad \bar{\sigma} t^{\prime}
$$

holds. Using the reflexivity rule of the Isabelle kernel we can start with the theorem $t \equiv t$ and then replay each $\tau$ reduction step using the Isabelle kernel operations, chaining them using the transitivity rule. For example, rule 3 of $\tau$ reduction in Definition 2.10 can be simulated using the instantiation of variables rule of the Isabelle kernel.

The only $\tau$ reduction step making trouble is $\eta$ abstraction. For an untyped term $s$ it is alright to go from $s$ to $\lambda\left(s \uparrow^{0} \cdot(\operatorname{Var} 0)\right)$, but for a welltyped Isabelle term $t$ such that $\delta=\operatorname{type}(t)$ is not of shape $\tau_{1} \rightarrow \tau_{2}$ this is not a valid step because it would lead to a term that is not welltyped any more. There is a workaround. We can just assume that everywhere in our proof so far the type $\delta$ has been replaced by the type unit $\rightarrow \delta$ and proceed replaying. We can do this because the type unit $\rightarrow \delta$ is isomorphic to $\delta$, so for each constant $c$ involving $\delta$ we could define a new constant

[^5]$c^{\prime}$ which behaves like $c$ but whose type is derived from that of $c$ by replacing $\delta$ by unit $\rightarrow \delta$.

This maybe not proves, but lets us very strongly believe:
The HCL cokernel is secure.
•Theorem 2.4

### 2.6.4 Mixing Modus Ponens, Instantiation, and Computation

Using the HCL cokernel comes with an overhead. Isabelle terms have to be converted into abstract machine terms for the purpose of computation, and after the computation has been performed, the resulting abstract machine terms have to be converted back to Isabelle terms. If the terms involved are big, the cost of converting between the Isabelle kernel and the cokernel universes can dominate the actual computing costs. In this subsection we scetch a simple feature of the HCL cokernel which drastically reduces traffic between kernel and cokernel and dramatically boosts performance in such a situation. The idea is that the cokernel assumes some reasoning responsibilities beyond computing equations.

Imagine an Isabelle theorem of the form:

$$
\begin{array}{cccc}
f_{1} & \equiv g_{1} \\
\Longrightarrow & f_{2} & \equiv & g_{2} \\
\Longrightarrow & f_{3} & \equiv & g_{3} \\
\vdots & \vdots & \vdots & \vdots \\
\Longrightarrow & f_{n} & \equiv & g_{n} \\
\Longrightarrow & \mathrm{p}
\end{array}
$$

One can understand such a theorem as an instruction book: First prove $f_{1} \equiv g_{1}$. Then prove $f_{2} \equiv g_{2}$. After that prove $f_{3} \equiv g_{3}$. When you have finally proved $f_{n} \equiv g_{n}$, you have proved the theorem $p$.

For the cokernel, proving means computing. So the instruction to prove $f_{1} \equiv g_{1}$ tells him to compute $f_{1}$ and $g_{1}$, and to get rid of the assumption $f_{1} \equiv g_{1}$ if both are equal. This brings together the logical rule of modus ponens with computation. If we furthermore throw in variable instantiation, the mix becomes really powerful. Typically the theorem will contain several variables. Some of these variables are used as template parameters; instantiating them means adapting the theorem to the situation at hand. After these template parameters have been instantiated, the values of the other variables will often be uniquely determined by the requirement that all assumptions $f_{i} \equiv g_{i}$ must be true.

Upon choosing an $i$, the cokernel will take the following actions:

1. Compute $f_{i}$ to $f_{i}^{\prime}$, and compute $g_{i}$ to $g_{i}^{\prime}$.
2. Try then to match $g_{i}^{\prime}$ with $f_{i}^{\prime}$ by instantiating the free variables in $g_{i}^{\prime}$ with terms which do not contain any of these free variables.
3. If this succeeds, remove the assumption $f_{i} \equiv g_{i}$ from the theorem and apply the found substitution throughout the whole theorem.

These actions are of course not executed on the Isabelle theorem, but on some theorem representation internal to the cokernel. The cokernel offers five securely accessible operations for this internal theorem representation:

1. Creation of an internal theorem from an Isabelle theorem.
2. Instantiation of variables of the internal theorem.
3. Elimination of assumptions of the internal theorem as described above.
4. Elimination of an assumption of the internal theorem by performing modus ponens with an Isabelle theorem. The assumptions of the Isabelle theorem are added as assumptions to the internal theorem.
5. Export of an internal theorem as an Isabelle theorem. This operation includes computing the proposition of the theorem as a whole before converting it into an Isabelle theorem.

The internal theorem is not represented by Isabelle terms, but is stored in the form of abstract machine terms. The substitutions involved in operation 2,3 and 4 are not executed directly, but delayed. This works very much like the closure mechanism of the Barras machine. Because the elements of the image of the substitutions are all closed abstract machine terms that have already been computed, they can be tagged with the Computed constructor when substituted into a term that is about to be evaluated.

### 2.6.5 Polymorphic Linking

Currently the HCL is not very user-friendly. The user has to gather all the theorems needed for computing himself. This situation is worsened considerably by the fact that the HCL cokernel performs no instantiations of type variables. For example, look at the If constant. For computing with it the two equations in (2.4) must be passed to the cokernel. But they have to be instantiated to exactly the type of the If constant they are supposed to work on. Now the If constant is used with quite a lot of different types, and it is unacceptable that the user has to provide all needed instantiations of equations (2.4).

Polymorphic linking solves this problem. The polymorphic linker is a wrapper around the cokernel. It allows to create a polymorphic computer which internally manages an ordinary computer. The polymorphic computer is created from a list of polymorphic theorems. When it is asked to compute a term it checks if new instances of these polymorphic theorems are needed and if so, updates the internal computer with those new theorems. The polymorphic computer provides the same interface as an ordinary computer. It also supports the feature presented in the previous subsection of mixing logical reasoning and computing.

## C H A P TER

## Proving Bounds for Real Linear Programs

The sky's the limit if you have a roof over your head.

- Sol Hurok


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### 3.1 Overview

In the next chapter our work will culminate in proving that about $92.5 \%$ of what we call the basic linear programs are infeasible. A prerequisite for this result is the
method of bounding the objective function of a linear program (LP) that we present in this chapter.

The method is due to Hales [12] where he describes how to obtain an arbitrarily precise upper bound for the maximum value of the objective function of an LP. Our contribution is to transfer this method into the rigid context of mechanical theorem provers, specifically our favorite one, Isabelle/HOL [25]. The burden of calculating the upper bound is delegated to an LP solver that needs not to be trusted. Instead, the LP solver delivers a small certificate to Isabelle/HOL that can be checked cheaply. Furthermore, there is no need to delve into the details of the actual method of optimizing an LP, which is usually the Simplex method. These details just do not matter for the theorem prover.

We first describe the basic idea of the method. Then we introduce the notion of finite matrices and explain why these are our representation of choice for linear programs. Finite matrices can be fitted into the system of numeric axiomatic type classes in Isabelle/HOL via the algebraic concept of lattice-ordered rings. Checking the certificate from the external LP solver is basically a calculation involving finite matrices. The matrices we have to deal with are sparse, therefore we introduce a sparse matrix representation of finite matrices.

We have presented most of the material in this chapter already in [26]. New additions are Sections 3.5, 3.7 and 3.8.

### 3.2 The Basic Idea

There are quite a lot of different ways to state a linear programming problem [32, sect. 7.4], which are all general in the sense that every linear programming problem can be stated that way. Here is one such way: a linear program consists of a matrix $A \in \mathbb{R}^{m \times n}$, a row vector $c \in \mathbb{R}^{1 \times n}$ and a column vector $b \in \mathbb{R}^{m \times 1}$. The goal is to maximize the objective function

$$
\begin{equation*}
x \longmapsto c x, \quad x \text { feasible }, \tag{3.1}
\end{equation*}
$$

where $x$ is called feasible iff $x \in \mathbb{R}^{n \times 1}$ and $A x \leq b$ holds. Note that we are dealing with matrix inequality here: $X \leq Y$ for two matrices $X$ and $Y$ iff every matrix element of $X$ is less than or equal to the corresponding element of $Y$.

Usually, the above stated goal really encompasses several goals / questions:

1. Find out if there exists any feasible $x$ at all (otherwise the LP is called infeasible).
2. Find out if there is a feasible $x_{\max }$ such that $c x_{\max } \geq c x$ for any feasible $x$, and calculate this $x_{\text {max }}$.
3. Calculate $M=\sup \{c x \mid x$ is feasible $\}$.

Note that $M=-\infty$ iff the answer to the first question is no. And $M=\infty$ iff the answer to the first question is yes and the answer to the second question is no. If $M<\infty$ then the LP is called bounded. Linear programming software is good at answering all those questions and at exhibiting (approximately) such an $x_{\max }$ if it exists. Our goal is more modest in some ways, but more demanding in others: assuming a priori bounds for the feasible region, that is assuming $l \leq x \leq u$ for all feasible $x$ with a priori known bounds $l$ and $u$, actually prove within Isabelle/HOL that $M \leq K$, where we can choose $K$ arbitrarily close to $M$. In particular, we do not want to calculate $x_{\max }$, but just want
to approximate $M$ as precise as we wish for. Furthermore, we can assume $M \neq \infty$ because of

$$
\begin{equation*}
M \leq \sum_{i=1}^{n}\left|c_{1 i}\right| \max \left\{\left|l_{i 1}\right|,\left|u_{i 1}\right|\right\}<\infty \tag{3.2}
\end{equation*}
$$

It might seem that our goal can be accomplished trivially by setting $K$ to the above sum. But of course this is not the case, as $K$ is probably not a particularly good approximation for $M$, and there is nothing in the above inequality telling us how to get a better approximation in case we need one.

### 3.2.1 Reducing the case $M=-\infty$ to the case $-\infty<M<\infty$

The case of an infeasible LP can be reduced to the case of a feasible LP [12]. We will give a more detailed description here than the one found in [12].

Remember that we are only considering LPs for which we know $l$ and $u$ s.t.

$$
\begin{equation*}
A x \leq b \Longrightarrow l \leq x \leq u \tag{3.3}
\end{equation*}
$$

In this subsection we additionally require $A$ to fulfill the inequality

$$
\begin{equation*}
A x \leq 0 \Longrightarrow x=0 \tag{3.4}
\end{equation*}
$$

This can easily be arranged by replacing $A$ and $b$ by $\tilde{A}$ and $\tilde{b}$ where

$$
\tilde{A}=\left(\begin{array}{c}
A  \tag{3.5}\\
I_{n} \\
-I_{n}
\end{array}\right) \quad \text { and } \quad \tilde{b}=\left(\begin{array}{c}
b \\
u \\
-l
\end{array}\right)
$$

$I_{n} \in \mathbb{R}^{n \times n}$ denotes the identity matrix.
Now let us assume that for the given LP both (3.3) and (3.4) hold. We can construct for any $K \in \mathbb{R}$ a modified LP with objective function

$$
\begin{equation*}
x^{\prime}=\binom{x}{t} \longmapsto c x+K t, \quad x^{\prime} \text { feasible, } \tag{3.6}
\end{equation*}
$$

where $x^{\prime} \in \mathbb{R}^{n+1}$ is called feasible with respect to the modified LP iff

$$
\begin{equation*}
A x+t b \leq b \quad \text { and } \quad 0 \leq t \leq 1 \tag{3.7}
\end{equation*}
$$

4 Theorem 3.1

On the left hand side of above equivalences we talk about feasibility with respect to the modified LP, on the right hand side about feasibility with respect to the original LP.

Proof. To show (3.8) in the direction from left to right one needs the fact that $A$ fulfills (3.4). The rest ist obvious by just expanding the respective definition of feasibility.

Theorem $3.2-$ Defining $M^{\prime}:=\sup \left\{c x+K t \left\lvert\, x^{\prime}=\binom{x}{t}\right., x^{\prime}\right.$ feasible $\}$ yields

$$
\begin{equation*}
-\infty<\max \{M, K\}=M^{\prime}<\infty \tag{3.10}
\end{equation*}
$$

As a special case follows

$$
\begin{equation*}
M=-\infty \Longrightarrow M^{\prime}=K \tag{3.11}
\end{equation*}
$$

Proof. Because of (3.8) we have $M^{\prime} \geq K$, in particular $M^{\prime}>-\infty$. Considering $t=0$ in (3.9) gives us $M^{\prime} \geq M$. From (3.9) and (3.3) in the case $t \neq 1$ and (3.8) in the case $t=1$ we obtain bounds for $x^{\prime}$ :

$$
x^{\prime}=\binom{x}{t} \text { is feasible } \Longrightarrow l^{-} \leq(1-t) l \leq x \leq(1-t) u \leq u^{+}
$$

Here $l^{-}$denotes the negative part of $l$ which results from $l$ by replacing every positive matrix element by 0 . Similarly, the positive part $u^{+}$results from $u$ by replacing every negative element by 0 . We conclude $M^{\prime}<\infty$.

So far we have shown $-\infty<\max \{M, K\} \leq M^{\prime}<\infty$. To complete the proof, we need to show $\max \{M, K\} \geq M^{\prime}$. We will proceed by case distinction.

Assume $M \geq K$. We show that for any feasible $x^{\prime}=\binom{x}{t}, M \geq c x+K t$, and therefore $M \geq M^{\prime}$. This is obvious in the case $t=1$, the feasibility of $x^{\prime}$ accompanied by the equivalence (3.8) forces $x$ to be zero. In the case $t \neq 1$, (3.9) implies that $x /(1-t)$ is feasible with respect to the original LP. But this is just what we claim:

$$
M \geq c(x /(1-t)) \Longrightarrow M \geq c x+t M \geq c x+t K
$$

Now assume $M<K$. Assume further $M^{\prime}>K$. Because of $-\infty<M^{\prime}<\infty$ there is a feasible $x^{\prime}=\binom{x}{t}$ s.t. $M^{\prime}=c x+K t$. For $t=1$ we would have again $x=0$ and therefore the contradiction $K<M^{\prime}=K$. Finally $0 \leq t<1$ also leads to a contradiction:

$$
M^{\prime}=c x+K t \leq c x+M^{\prime} t \Longrightarrow M^{\prime} \leq c(x /(1-t)) \leq M<K \leq M^{\prime}
$$

Therefore the only possibility is $M^{\prime} \leq K$.
From now on we will assume that we are dealing with feasible, bounded LPs, that is with LPs for which we know $-\infty<M<\infty$.

### 3.2.2 The case $-\infty<M<\infty$

This case is the heart of the method. Again we construct a modified LP. The original LP is called the primal LP, the modified LP is called the dual LP. The objective function of the dual LP

$$
y \longmapsto y b, \quad y \text { feasible, }
$$

is to be minimized. Here $y \in \mathbb{R}^{1 \times m}$ is called feasible iff $y A=c$ and $y \geq 0$ holds.
Theorem $3.3-$ Any feasible $y$ induces an upper bound on $M$ :

$$
\begin{equation*}
y b \geq M \tag{3.12}
\end{equation*}
$$

Proof. For any feasible $x$ we have

$$
\begin{equation*}
y b \geq y(A x)=(y A) x=c x . \tag{3.13}
\end{equation*}
$$

But is there such a feasible $y$ so that we can utilize (3.12)? And if there is, can we accomplish $y b=M$ by carefully choosing $y$ ? The well-known answer to both questions is yes:
Define $M^{\prime}:=\inf \{y b \mid y A=c$ and $y \geq 0\}$. Then

$$
\begin{equation*}
-\infty<M=M^{\prime}<\infty \tag{3.14}
\end{equation*}
$$

Furthermore, choose a feasible $y$ such that $M^{\prime}=y b$. Then

$$
\begin{equation*}
\operatorname{card}\left\{i \in \mathbb{N} \mid 1 \leq i \leq m \text { and } y_{1 i}>0\right\} \leq n \tag{3.15}
\end{equation*}
$$

Proof. Corollary 7.1g and 7.11 in [32].
Now the basic idea of our method can be described as follows. First, form the dual LP. Then use an external LP solver to solve the dual LP for an optimal $y$. This optimal $y$ serves as a certificate. In our application, where typically $m \approx 2000$ and $n \approx 200, y$ will be sparse, as inequality (3.15) tells us. Finally, use (3.12) to verify our desired upper bound $M \leq K=y b$.

This basic idea is complicated by the fact that we are dealing with real data and numerical algorithms. The external LP solver does not return an $y$ such that $y A=c$ and $y \geq 0$, but rather an $y$ such that $y A \approx c$ and $y \gtrsim 0$. In order to obtain a provably upper bound on $M$, one has to take (3.3) into account. Furthermore the input data $A$, $b$ and $c$ need not to be given as exact numerical data either, for example an element of $A$ could equal $\pi$. The way to deal with these complications is to use interval arithmetic, not only for real numbers, but also for real matrices.

### 3.3 Finite Matrices

Anyone who wants to implement the method outlined in the previous section faces the problem of how to represent linear programs. This problem is prominent outside of the realm of mechanical theorem proving, too: designers of linear programming packages typically provide various ways of input of data to the LP algorithms these packages provide, one can normally choose at least between dense and sparse representations of the data. The issue is to provide a certain convenience of dealing with the data without compromising the efficiency of the LP algorithms by too much overhead.

Our situation is different: we need to reason within our mechanical theorem proving environment Isabelle/HOL why our computations lead to a correct result, therefore we need a good representation of LPs for reasoning about them. Of course we also need to compute efficiently. But we should avoid mixing up those two issues if we can. The reasoning in the previous section has used matrices and the properties of matrix operations like associativity of matrix multiplication extensively. Therefore representing LPs within Isabelle/HOL as matrices is a good idea.

So how exactly does one represent matrices in higher-order logic? Obviously, matrices should be a type, but how does one deal with the dimension of a matrix? HOL does not have dependent types, so it seems impossible to have a parametrized family of types where the dimension of the matrix would be the parameter. But it is: one possibility that is pursued by John Harrison in the 2005 version of his Hollight system is to represent the needed parameter by type variables! He uses this representation in order to formalize multivariate calculus. But in our case this idea cannot be used without causing serious problems later when we turn our attention to sparse matrices.

Another possibility is to represent the dimension of a matrix by a predicate that carves the set of all matrices of this dimension out of a certain bigger, already existing type. This is a common technique to overcome the absence of dependent types in HOL [18]. This approach could work like this: ${ }^{1}$

```
type \(\alpha M=\) nat \(\times\) nat \(\times(\) nat \(\Rightarrow\) nat \(\Rightarrow \alpha)\)
constdef
    Mequiv :: \((\alpha M * \alpha M)\) set
    Mequiv \(\equiv\{((m, n, f),(m, n, g)) \mid \forall j i .(j<m \wedge i<n) \longrightarrow f j i=g j i\}\)
typedef \(\alpha\) matrix \(=\) UNIV // Mequiv
```

constdef
is-matrix :: nat $\Rightarrow$ nat $\Rightarrow \alpha$ matrix $\Rightarrow$ bool
is-matrix $m n A \equiv \exists f$. $(m, n, f) \in$ Rep-matrix $A$.

In (3.16) $\alpha$ matrix is the bigger type, and is-matrix $m n$ acts as the predicate that carves out all matrices consisting of $m$ rows and $n$ columns. Here matrices are modelled as equivalence classes [31] of triples ( $m, n, f$ ) where $m$ denotes the number of rows, $n$ the number of columns and $f$ a function from indices to matrix elements. The set of these equivalence classes is denoted by UNIV // Mequiv. With this formalization of matrices an error element comes for free: there is exactly one matrix Error such that
is-matrix00 Error
holds. When adding matrices $A$ and $B$ which fulfill

$$
\begin{equation*}
\exists m n \cdot(\text { is-matrix } m n A) \wedge(\neg \text { is-matrix } m n B) \tag{3.18}
\end{equation*}
$$

and when multiplying matrices $A$ and $B$ for which

$$
\begin{equation*}
\exists m n u v .(\text { is-matrix } m n A) \wedge(\text { is-matrix } u v B) \wedge(n \neq u) \tag{3.19}
\end{equation*}
$$

holds, the matrix Error is returned to signal that the operands do not belong to the natural domain of addition and multiplication, respectively.

Still, this approach is not entirely satisfying: in Isabelle/HOL there exists a large number of theorems that are valid for types that form a group or a ring. The fact that a type can be viewed as such an algebraic structure is formulated via the concept of

[^6]axiomatic type classes [30]. But $\alpha$ matrix in (3.16) with the suggested error signaling definition of addition does not even form a group, because there is no matrix Zero with
\[

$$
\begin{equation*}
\forall A \cdot A+\text { Zero }=A \tag{3.20}
\end{equation*}
$$

\]

but rather a whole family Zeromn such that

$$
\begin{equation*}
\forall A \text {.is-matrixmn } A \longrightarrow A+(\text { Zeromn })=A . \tag{3.21}
\end{equation*}
$$

Therefore we advocate a different approach that exploits the fact that the matrix elements commonly used in mathematics [20] themselves carry an algebraic structure, that of a ring, which always contains a zero. We define $\alpha$ matrix to be the type formed by all infinite matrices that have only finitely many non-zero elements of type $\alpha$ :

$$
\begin{align*}
& \text { type } \alpha \text { infmatrix }=\text { nat } \Rightarrow \text { nat } \Rightarrow \alpha \\
& \text { typedef } \alpha \text { matrix }=\{f::(\alpha:: \text { zero) infmatrix } \mid \text { finite }\{(j, i) \mid f j i \neq 0\}\} . \tag{3.22}
\end{align*}
$$

Hence we choose the name finite matrices for objects of type $\alpha$ matrix. Note the restriction $\alpha::$ zero in (3.22). This means that the elements of a matrix cannot have just any type but only a type that is an instance of the axiomatic type class zero and has thus an element denoted by 0 . Of course this is not a real restriction on the type; any type can be declared to be an instance of the axiomatic type class zero.

### 3.3.1 Dimension of a Finite Matrix

The dimension of a finite matrix deviates from the notion of dimension that one is used to. Because we did not encode the number of rows and columns explicitly in the representation of a finite matrix as we did in (3.16), we have to recover the dimension of a finite matrix by extensionality:

```
constdefs
    nrows :: \alpha matrix }=>\mathrm{ nat
    nrows A =LEASTm. }\forall\mathrm{ ji.m }\leqj\longrightarrow(\mathrm{ Rep-matrix A ji=0)
    ncols :: \alpha matrix }=>\mathrm{ nat
    ncols A =LEASTn.\forallji.n\leqi\longrightarrow(Rep-matrix Aji=0)
    is-matrix :: nat }=>\mathrm{ nat }=>\alpha\mathrm{ matrix }=>\mathrm{ bool
    is-matrix m n A = nrows }A\leqm\wedge ncols A\leqn .
```

The expression LEAST $x$.P $x$ equals the least $x$ such that $P x$ holds. The definition of the type $\alpha$ matrix has introduced two automatically defined functions Rep-matrix and Abs-matrix

```
consts
    Rep-matrix :: \alpha matrix }=>\alpha\mathrm{ infmatrix
    Abs-matrix :: }\alpha\mathrm{ infmatrix }=>\alpha\mathrm{ matrix
```

that convert between finite matrices and infinite matrices. They enjoy the following crucial properties:

$$
\begin{align*}
& (A=B)=(\forall j i . \text { Rep-matrix } A j i=\text { Rep-matrix } B j i),  \tag{3.25}\\
& \exists_{1} f . A=A b s \text {-matrix } f, \tag{3.26}
\end{align*}
$$

$$
\begin{align*}
& \text { Abs-matrix }(\text { Rep-matrix } A)=A  \tag{3.27}\\
& \text { finite }\{(j, i) \mid \operatorname{Rep} \text {-matrix } A j i \neq 0\}  \tag{3.28}\\
& \text { finite }\{(j, i) \mid f j i \neq 0\} \Longrightarrow \operatorname{Rep} \text {-matrix }(\text { Abs-matrix } f)=f \tag{3.29}
\end{align*}
$$

Thus Rep-matrix $A j i$ denotes the matrix element of $A$ in row $j$ and column $i$. Note that the first row is row 0 , likewise for columns.

Let us return to the definitions in (3.23). The definition of is-matrix implies that a matrix has not exactly one dimension, but infinitely many! Therefore there is no need for signaling an error due to incompatibility of dimensions: for any two matrices $A$ and $B$ one shows
$\exists$ m.is-matrix $m m A \wedge$ is-matrix $m m B$.
The intuition behind (3.30) is that every matrix can be viewed as a square matrix of dimension $m$ as long as $m$ is large enough: one just needs to fill up the missing rows and columns with zeros.

The need for an Error matrix has vanished, but one can still use (3.17) to uniquely define a matrix. This time, we denote that matrix by 0 :

$$
\begin{equation*}
\forall A .(A=0)=(\text { is-matrix } 00 A) . \tag{3.31}
\end{equation*}
$$

Another possibility of defining 0 is given by the following theorem:

$$
\begin{equation*}
\forall A .(A=0)=(\forall m n \text {.is-matrixmn } A) . \tag{3.32}
\end{equation*}
$$

We will see that 0 is actually the proper name for this matrix.

### 3.3.2 Lifting Unary Operators

In this subsection we look at how to define an unary operator $U$ on matrices,

$$
\begin{equation*}
U:: \alpha \text { matrix } \Rightarrow \beta \text { matrix } \tag{3.33}
\end{equation*}
$$

by lifting an unary operator $u$ on matrix elements,

$$
\begin{equation*}
u:: \alpha \Rightarrow \beta . \tag{3.34}
\end{equation*}
$$

The first step is to lift $u$ to infinite matrices:

```
constdef
    apply-infmatrix :: (\alpha=>\beta)=>(\alpha infmatrix }=>\beta\mathrm{ infmatrix)
    apply-infmatrix u}\equiv\lambdafji.u(fji)
```

which results in the lifting property

$$
\begin{equation*}
\text { (apply-infmatrixu f) } j i=u(f j i) . \tag{3.36}
\end{equation*}
$$

Its proof is apparent from the definition of apply-infmatrix.
Now the unary lifting operator apply-matrix can be defined by first lifting $u$ to infinite matrices, and then to finite matrices:

```
constdef
    apply-matrix :: (\alpha=>\beta)=>(\alpha matrix }=>\beta\mathrm{ matrix)
    apply-matrix }u\equiv\lambdaA\mathrm{ .Abs-matrix(apply-infmatrixu(Rep-matrix A)) .
```

What is the lifting property for apply-matrix? A first guess yields
Rep-matrix $($ apply-matrix $u A) j i=u($ Rep-matrix $A j i)$.
But this is false (in the sense that we cannot prove it in HOL)! To see why, consider $\alpha=\beta=$ int and $u=\lambda x .1$. Then we have

$$
\text { apply-infmatrix } u(\text { Rep-matrix } A)=\left(\begin{array}{ccc}
1 & 1 & \cdots  \tag{3.39}\\
1 & 1 & \cdots \\
\vdots & \vdots & \ddots
\end{array}\right) \neq \operatorname{Rep}-\text { matrix } B
$$

for all matrices $A$ and any matrix $B$. But there is a simple condition on $u$ that turns out to be sufficient and necessary to prove (3.38):

$$
\begin{equation*}
u 0=0 \Longrightarrow \operatorname{Rep} \text {-matrix }(\text { apply-matrix } u A) j i=u(\text { Rep-matrix } A j i) . \tag{3.40}
\end{equation*}
$$

This is easily provable using (3.37), (3.28), (3.29) and (3.36).

### 3.3.3 Lifting Binary Operators

Just as we have defined a unary lifting operator apply-matrix, we can define similarly a binary lifting operator combine-matrix:

```
constdef
    combine-infmatrix ::
        (\alpha=>\beta=>\gamma)=>(\alpha infmatrix }=>\beta\mathrm{ infmatrix }=>\gamma\mathrm{ infmatrix)
    combine-infmatrix v\equiv\lambdafgji.v(fji)(gji),
constdef
    combine-matrix :: (\alpha=>\beta=>\gamma)=>(\alpha matrix }=>\beta\mathrm{ matrix }=>\gamma\mathrm{ matrix }
    combine-matrix v \equiv
        \lambdaAB.Abs-matrix(combine-infmatrixv(Rep-matrixA)(Rep-matrix B)),
```

The lifting property for combine-matrix reads

$$
v 00=0 \Longrightarrow \underset{v(\text { Rep-matrix } A j i)(\text { Rep-matrix } B j i)}{\text { Rep-matrix }(\text { combine-matrix } A B)} .
$$

Lifting binary operators passes on commutativity and associativity. Defining

```
constdefs
    commutative :: (\alpha=>\alpha=>\beta)=> bool
    commutative v}\equiv\forallxy.vxy=vy
    associative:: ( }\alpha=>\alpha=>\alpha)=>\mathrm{ bool
    associative v\equiv\forallxyz.v(vxy)z=vx(vyz)
associative \(v \equiv \forall x y z . v(v x y) z=v x(v y z)\)
```

we can formulate this propagation concisely:
commutativev $\Longrightarrow$ commutative (combine-matrixv),
$\llbracket v 00=0 ;$ associativev $\rrbracket \Longrightarrow$ associative (combine-matrixv) .
You might be surprised that the propagation of commutativity does not require $v 00=0$, which is due to the idiosyncrasies of the definite description operator that is hidden in Abs-matrix.

### 3.3.4 Matrix Multiplication

We need one last lifting operation, the most interesting one: given two binary operators addition and multiplication on the matrix elements, define the matrix product induced by those two operators. As a basic tool we first define by primitive recursion a fold operator that acts on sequences:

```
const foldseq \(::(\alpha \Rightarrow \alpha \Rightarrow \alpha) \Rightarrow(\) nat \(\Rightarrow \alpha) \Rightarrow\) nat \(\Rightarrow \alpha\)
primrec
    foldseq f s \(0=s 0\)
    foldseq \(f s(\) Sucn \()=f(s 0)(\) foldseq \(f(\lambda k . s(\) Suck \()) n)\)
```

For illustration purposes, assume $s=\left(s_{1}, s_{2}, s_{3}, s_{4}, \ldots, s_{n}, 0,0,0, \ldots\right)$. Then

```
foldseq f s 0 = s ,
foldseq f s 1 = fs s s 2,
foldseq fs 2=fs ( }f\mp@subsup{s}{2}{}\mp@subsup{s}{3}{})\mathrm{ ),
foldseq fs s =fs ( }(f\mp@subsup{s}{2}{}(f\mp@subsup{s}{3}{}\mp@subsup{s}{4}{}))
foldseq fs n =fs s}(f\mp@subsup{s}{2}{}(\ldots(f\mp@subsup{s}{n}{}0)\ldots..))
foldseq fs(n+1)=fs
```

Note that if $f 00=0$ the above sequence converges:

$$
\begin{equation*}
f 00=0 \Longrightarrow \forall m \cdot n \leq m \longrightarrow \text { foldseq } f s m=\text { foldseq } f s n . \tag{3.48}
\end{equation*}
$$

Now we are prepared to deal with matrix multiplication:

```
constdef
    mult-matrix-n :: nat }=>(\alpha=>\beta=>\gamma)=>(\gamma=>\gamma=>\gamma)
                    \alpha matrix }=>\beta\mathrm{ matrix }=>\gamma\mathrm{ matrix
    mult-matrix-n n mult add A B = Abs-matrix ( }\lambda\mathrm{ ji.
        foldseqadd( }\lambdak\mathrm{ .mult(Rep-matrixA jk)(Rep-matrixBki))n)
```

The idea of mult-matrix-nn multadd $A B$ is to consider only the first $n$ columns of $A$ and the first $n$ rows of $B$ when calculating the matrix product. Of course the matrix product should be independent of $n$. We achieve this by setting

$$
\begin{equation*}
\text { mult-matrix multadd } \equiv \lim _{n \rightarrow \infty} \text { mult-matrix-n } n \text { multadd }, \tag{3.50}
\end{equation*}
$$

which is due to (3.48) well-defined if $\forall x$. mult $x 0=\operatorname{mult} 0 x=\operatorname{add} 00=0$ holds:

```
constdef
    mult-matrix :: (\alpha=>\beta=>\gamma)=>(\gamma=>\gamma=>\gamma)=>
                \alpha matrix }=>\beta\mathrm{ matrix }=>\gamma\mathrm{ matrix
    mult-matrix mult add A B \equiv
        mult-matrix-n(max(ncolsA)(nrowsB)) multadd A B .
```

Again, we have a lifting property:

$$
\begin{align*}
& \llbracket \forall x . \text { mult } x 0=0 \wedge \text { mult } 0 x=0 ; \text { add } 00=0 \rrbracket \Longrightarrow \\
& \quad \text { Rep-matrix }(\text { mult-matrix multadd } A B) j i=\text { foldseqadd }  \tag{3.52}\\
& \quad(\lambda k . \text { mult }(\text { Rep-matrixA } j k)(\text { Rep-matrix Bki) })(\max (\text { ncols } A)(\text { nrows } B)) .
\end{align*}
$$

Finally, let us examine what properties of element addition and element multiplication induce distributivity and associativity of mult-matrix.

### 3.3.4.1 Distributivity

We distinguish between left and right distributivity: ${ }^{2}$

```
constdefs
    r-distributive :: \((\alpha \Rightarrow \beta \Rightarrow \beta) \Rightarrow(\beta \Rightarrow \beta \Rightarrow \beta) \Rightarrow\) bool
    \(r\)-distributive mult add \(\equiv \forall\) auv.multa \((\) adduv \()=\) add (multau) (multav) \(\quad\) - \(\quad\) (3.53)
distributive \(:: ~(\alpha \Rightarrow \beta \Rightarrow \alpha) \Rightarrow(\alpha \Rightarrow \alpha \Rightarrow \alpha) \Rightarrow\) bool
    l-distributive mult add \(\equiv \forall\) auv.mult(adduv) \(a=\operatorname{add}(\) multua) (multva)
```

Distributivity of mult over add lifts to distributivity of mult-matrix mult add over combine-matrix add if add is associative and commutative and both add and mult behave as expected with respect to 0 :

【l-distributive mult add; associative add; commutative add;
$\forall x$. multx $0=0 \wedge$ mult $0 x=0 ;$ add $00=0 \rrbracket$
$\Longrightarrow 1$-distributive (mult-matrix mult add) (combine-matrix add),
【 $r$-distributive mult add; associative add; commutative add;
$\forall x$. multx $0=0 \wedge$ mult $0 x=0 ;$ add $00=0 \rrbracket$
$\Longrightarrow r$-distributive (mult-matrix mult add) (combine-matrix add) .

### 3.3.4.2 Associativity

We state the law of associativity for mult-matrix in a very general form:
$\llbracket \forall a$. mult $_{1} a 0=0 ; \forall a$. mult $_{1} 0 a=0 ; \forall a$. mult $_{2} a 0=0 ; \forall a$. mult $_{2} 0 a=0$; $\operatorname{add}_{1} 00=0 ; \operatorname{add}_{2} 00=0$; $\forall a b c d . a d d_{2}\left(a d d_{1} a b\right)\left(a d d_{1} c d\right)=\operatorname{add}_{1}\left(a d d_{2} a c\right)\left(a d d_{2} b d\right)$;
$\forall a b c$. mult $_{2}\left(\right.$ mult $\left._{1} a b\right) c=$ mult $_{1} a\left(\right.$ mult $\left._{2} b c\right)$;
associative add ${ }_{1}$; associative add ${ }_{2}$;
l-distributive mult add $_{1} ;$ r-distributive mult add $_{2} \mathbb{I}$
$\Longrightarrow$ mult-matrix mult add $_{2}$ (mult-matrix mult add $_{1} A B$ ) $C=$ mult-matrix mult add $_{1} A$ (mult-matrix mult add $_{2} B C$ ).

For mult $=$ mult $_{1}=$ mult $_{2}$ and add $=$ add $_{1}=$ add $d_{2}$ this simplifies to
$\llbracket \forall a \cdot$ multa $0=0 ; \forall a \cdot$ mult $0 a=0 ;$ add $00=0 ;$
associative add; commutative add; associative mult;
l-distributive mult add; r-distributive mult add $\rrbracket$
$\Longrightarrow$ associative (mult-matrix mult add) .

### 3.3.5 Lattice-Ordered Rings

Paulson describes in [30] how numerical theories like the theory of integers or the theory of reals can be organized in Isabelle/HOL using axiomatic type classes. For example both integers and reals form a ring, therefore Paulson recommends to prove theorems that are implied purely by ring properties only once, and then to prove that both types int and the type real are an instance of the axiomatic type class ring.

Birkhoff points out [4, chapt. 17] that for a fixed $n$ the ring of all $n \times n$ square matrices forms a latticed-ordered ring in a natural way. The same is true for our finite matrices! Therefore it suggests itself to establish an axiomatic type class lordered-ring that captures the property of a type to form a lattice-ordered ring. Of

[^7]course lordered-ring should be integrated with the other type classes like ring and ordered-ring of Isabelle/HOL to maximize theorem reuse. Two major changes along with minor modifications were necessary to the original hierarchy of type classes as described in [30]:

1. The original type class ring demanded both the existence of a multiplicative unit element and the commutativity of multiplication. But our finite matrices do not have such a multiplicative unit element, nor is multiplication of finite matrices a commutative operator. Nevertheless, finite matrices still form a ring in common mathematical terminology. Therefore the original type class ring was renamed to become comm-ring-1 and new type classes ring, ring-1 and comm-ring were introduced, suitable for rings that do not necessarily possess a 1 and/or are not commutative.
2. All ordered algebraic structures contained in the original hierarchy were linearly ordered. The natural (elementwise) order for finite matrices is a proper partial order, actually a lattice order. Therefore we enriched the hierarchy with type classes that model partially ordered algebraic systems like partially ordered groups and rings, or lattice-ordered groups and rings. For this we follow largely [7], [4].

A type $\alpha$ is an instance of the axiomatic type class lordered-ring iff
ring $\alpha$ is a ring with addition + , subtraction - , additive inverse - , multiplication *, zero 0,
lattice $\alpha$ is a lattice with partial order $\leq$ and operators join and meet,
monotonicity addition and multiplication are monotone:

$$
\begin{gather*}
a \leq b \longrightarrow c+a \leq c+b,  \tag{3.57}\\
a \leq b \wedge 0 \leq c \longrightarrow a * c \leq b * c \wedge c * a \leq c * b . \tag{3.58}
\end{gather*}
$$

Both int and real are instances of lordered-ring:
instance int :: lordered-ring
instance real :: lordered-ring .
Our goal is to prove
instance matrix :: (lordered-ring) lordered-ring .
The above meta theorem has the following meaning (which is not legal Isabelle syntax):

$$
\begin{equation*}
\text { (instance } \alpha:: \text { lordered-ring) } \Longrightarrow \text { (instance } \alpha \text { matrix :: lordered-ring) . } \tag{3.61}
\end{equation*}
$$

Of course, in order to prove (3.60), one first has to define $0,+, *$ etc. for objects of type matrix. The zero matrix is easy to define:

```
instance matrix :: (zero) zero
def (overloaded)
    0\equivAbs-matrix(\lambdaji.0) .
```

It is simple to show that this is actually the 0 we refer to in (3.31) and (3.32).

Addition + , multiplication *, subtraction -, unary minus -, can all be defined using the lifting machinery we have developed:

```
instance matrix :: (plus) plus
instance matrix :: (minus) minus
instance matrix :: ({plus, times}) times
defs (overloaded)
    A+B \equiv combine-matrix (\lambdaab.a+b)AB
    A-B \equiv combine-matrix(\lambdaab.a-b)AB
        -A \equivapply-matrix(\lambdaa.-a)A
    A*B \equiv mult-matrix(\lambdaab.a*b)(\lambdaab.a+b)AB.
```

Finally, we need to be able to compare matrices:

```
instance matrix :: ({ord, zero}) ord
defs (overloaded)
    A\leqB\equiv}\equiv\forallji.Rep-matrixAji\leqRep-matrix Bji
```

After having introduced the necessary syntax, we need to show that $\alpha$ matrix really constitutes a lattice-ordered ring, provided $\alpha$ constitutes one, in order to obtain (3.60). But almost the entire work has already been done: for example, in order to prove associativity of matrix multiplication,

$$
\begin{equation*}
\forall(A::(\alpha:: \text { lordered-ring }) \text { matrix }) \cdot A *(B * C)=(A * B) * C, \tag{3.65}
\end{equation*}
$$

which is the hardest of all proof obligations, just apply (3.56)! The remaining proof obligations are not difficult to prove, either, one just has to make use of matrix extensionality (3.25) and the lifting properties (3.40), (3.43) and (3.52). It is useful, though, first to dispose of the assumptions in these lifting properties, so for example instead of using (3.43) directly one should prove and use

$$
\begin{align*}
& \text { Rep-matrix }(A+B) j i=(\text { Rep-matrix } A j i)+(\operatorname{Rep}-\text { matrix } B j i) \\
& \operatorname{Rep-matrix}(A-B) j i=(\text { Rep-matrix } A j i)-(\operatorname{Rep}-\text { matrix } B j) . \tag{3.66}
\end{align*}
$$

A proof obligation that differs from the others because it is not a universal property that needs to be shown, but an existential one, turns up when one has to show that join and meet do exist:

$$
\begin{align*}
& \exists j . \forall a b x . a \leq j a b \wedge b \leq j a b \wedge(a \leq x \wedge b \leq x \longrightarrow j a b \leq x) \\
& \exists m . \forall a b x . m a b \leq a \wedge m a b \leq b \wedge(x \leq a \wedge x \leq b \longrightarrow x \leq m a b) \tag{3.67}
\end{align*}
$$

But these are not difficult to exhibit! Just choose

$$
\begin{equation*}
\text { join } \equiv \text { combine-matrix join, meet } \equiv \text { combine-matrix meet } . \tag{3.68}
\end{equation*}
$$

### 3.3.6 Positive Part and Negative Part

In lattice-ordered rings (actually in groups, also), both the positive part and the negative part can be defined:

```
constdefs
    pprt :: \alpha=> (\alpha :: lordered-ring)
    pprt x \equivjoinx0
    nprt :: \alpha ( }\alpha:: lordered-ring
    nprt x \equiv meetx 0
```

We will write $x^{+}$instead of pprtx, and $x^{-}$instead of nprtx. We have:

$$
\begin{equation*}
0 \leq x^{+}, \quad x^{-} \leq 0, \quad x=x^{+}+x^{-}, \quad x \leq y \Longrightarrow x^{-} \leq y^{-} \wedge x^{+} \leq y^{+} . \tag{3.70}
\end{equation*}
$$

Positive part and negative part come in handy for calculating bounds for a product when bounds for each of the factors of the product are known:

$$
\begin{align*}
& \llbracket a_{1} \leq a ; a \leq a_{2} ; b_{1} \leq b ; b \leq b_{2} \rrbracket \\
& \Longrightarrow a * b \leq a_{2}^{+} * b_{2}^{+}+a_{1}^{+} * b_{2}^{-}+a_{2}^{-} * b_{1}^{+}+a_{1}^{-} * b_{1}^{-} \tag{3.71}
\end{align*}
$$

In order to prove (3.71), decompose the factors into their parts and use distributivity. Then take advantage of the monotonicity of positive and negative part:

$$
\begin{aligned}
a * b & =\left(a^{+}+a^{-}\right) *\left(b^{+}+b^{-}\right) \\
& =a^{+} * b^{+}+a^{+} * b^{-}+a^{-} * b^{+}+a^{-} * b^{-} \\
& \leq a_{2}^{+} * b_{2}^{+}+a_{1}^{+} * b_{2}^{-}+a_{2}^{-} * b_{1}^{+}+a_{1}^{-} * b_{1}^{-} .
\end{aligned}
$$

### 3.4 Proving Bounds by Duality

Now we have everything in place to represent LPs by finite matrices. In sect. 3.2, we presented the basic idea of how to prove an arbitrarily precise upper bound for the objective function (3.1) of a given LP. There the LP was represented by matrices whose elements are real numbers:

$$
c \in \mathbb{R}^{1 \times n}, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^{m \times 1}, \quad l, u \in \mathbb{R}^{n \times 1} \text {. }
$$

Dropping the dimensions we arrive at a representation of a real linear program by finite matrices:

$$
c, A, b, l, u:: \text { real matrix . }
$$

From now on we are always talking in terms of finite matrices.
We need a further modification of our representation of LPs: our method is based on numerical algorithms like the Simplex method, therefore we need to represent the data numerically. We allow for this possibility by looking at intervals of linear programs instead of only considering a single LP. Such an interval is given by finite matrices $c_{1}, c_{2}, A_{1}, A_{2}, b, l, u$. We can now state the main theorem as it has been proven in Isabelle/HOL:

$$
\begin{gather*}
\llbracket A * x \leq b ; A_{1} \leq A ; A \leq A_{2} ; c_{1} \leq c ; c \leq c_{2} ; l \leq x ; x \leq u ; 0 \leq y \rrbracket \\
\Longrightarrow c * x \leq y * b+\left(\operatorname{let} s_{1}=c_{1}-y * A_{2} ; s_{2}=c_{2}-y * A_{1}\right.  \tag{3.72}\\
\text { in } \left.s_{2}^{+} * u^{+}+s_{1}^{+} * u^{-}+s_{2}^{-} * l^{+}+s_{1}^{-} * l^{-}\right) .
\end{gather*}
$$

The proof is by standard algebraic manipulations: using $A * x \leq b$ and $y \geq 0$,

$$
c * x \leq y * b+(c-y * A) * x
$$

follows at once. Then one just has to apply (3.71) to the product $(c-y * A) * x$. Note that this proof not only works for matrices, but for any lattice-ordered ring. Therefore the main theorem is valid also for lattice-ordered rings!

This is how our method works: First, we calculate the approximate optimal solution $y$ of the dual LP. We know our primal LP only approximately, so we can pass only approximate data to the external LP solver. We could pass for example $c_{1}$,
$A_{1}, b, l, u$. The LP solver will return the certificate $y$, which is only approximately non-negative. Therefore we replace all negative elements of $y$ by 0 . We then plug the known numerical data $y, c_{1}, c_{2}, A_{1}, A_{2}, b, l$ and $u$ into (3.72) and simplify the resulting theorem. The simplification will rewrite $0 \leq y$ to True and the large expression on the right hand side of the inequality to a matrix numeral $K$ with ncols $K \leq 1$ and nrows $K \leq 1$. The result of our method is therefore the theorem

$$
\begin{align*}
& \llbracket \boldsymbol{A} * \boldsymbol{x} \leq b ; A_{1} \leq \boldsymbol{A} ; \boldsymbol{A} \leq A_{2} ; c_{1} \leq \boldsymbol{c} ; \boldsymbol{c} \leq c_{2} ; l \leq \boldsymbol{x} ; \boldsymbol{x} \leq u \rrbracket  \tag{3.73}\\
& \Longrightarrow \boldsymbol{c} * \boldsymbol{x} \leq K .
\end{align*}
$$

In the above theorem, free variables are set in bold face. All other identifiers denote matrix numerals.

### 3.5 Proving Infeasibility by Modified Duality

If our linear program at hand is infeasible, the method of Section 3.4 will fail because the dual program will also be infeasible and the external solver will fail. How do we prove a bound of an infeasible linear program then? We have outlined the basic idea of how to do this already in Section 3.2.1. We take the infeasible linear program and modify it so that we get a new, feasible linear program. We then apply the method from Section 3.4 to bound this new linear program. Then we somehow find a way to relate the found bound of the new linear program to a bound for the original one according to Theorem 3.2.

Our original linear program is:
Maximize $c * x$ where $x$ is subject to the condition $A * x \leq b$.
For any $K$ the modified linear program is to maximize $c * x+K * t$ subject to the condition $A * x+b * t \leq b$ and $0 \leq t \leq 1$. We can squeeze the modified linear program into standard form so that it becomes:

$$
\text { Maximize } c^{\prime} * x^{\prime} \text { where } x^{\prime} \text { is subject to the condition } A^{\prime} * x^{\prime} \leq b^{\prime}
$$

where

$$
c^{\prime}=\left(\begin{array}{ll}
c & K
\end{array}\right), \quad x^{\prime}=\binom{x}{t}, \quad A^{\prime}=\left(\begin{array}{cc}
A & b \\
0 & 1 \\
0 & -1
\end{array}\right), \quad b^{\prime}=\left(\begin{array}{l}
b \\
1 \\
0
\end{array}\right) .
$$

Now let's do for this modified linear program what we always do for a feasible linear program: solve the dual linear program and get a certificate $y^{\prime}$. Because $A^{\prime}$ has two more rows than $A$, we can write $y^{\prime}$ as $y^{\prime}=\left(\begin{array}{lll}y & y_{1} & y_{2}\end{array}\right)$ for some vector $y \geq 0$ and numbers $y_{1} \geq 0, y_{2} \geq 0$. If the original LP is infeasible, Theorem 3.2 implies

$$
c^{\prime} * x^{\prime} \leq y^{\prime} * b^{\prime} \approx K
$$

As this holds for any $x^{\prime}$, we can just as well choose an $x^{\prime}=\binom{x}{t}$ such that $t=0$ :

$$
c * x=c^{\prime} *\binom{x}{0} \leq y^{\prime} * b^{\prime}=\left(\begin{array}{lll}
y & y_{1} & y_{2}
\end{array}\right) *\left(\begin{array}{l}
b \\
1 \\
0
\end{array}\right)=y * b+y_{1} * 1+y_{2} * 0=y * b+y_{1} \approx K .
$$

This looks terrific, because it bounds the objective function $c * x$ of the original linear program by $y * b+y_{1}$ which depends on the certificate of the modified linear program! Furthermore, because $K$ was chosen arbitrarily, we can push the bound for $c * x$ as low as we want to. And the best thing is that we do not even need to prove any fancy new theorem for using this fact! The theorem

$$
\begin{gather*}
\llbracket A * x \leq b ; A_{1} \leq A ; A \leq A_{2} ; c_{1} \leq c ; c \leq c_{2} ; l \leq x ; x \leq u ; 0 \leq y ; 0 \leq y_{1} \rrbracket \\
\Longrightarrow c * x \leq y * b+y_{1}+\left(\operatorname{let} s_{1}=c_{1}-y * A_{2} ; s_{2}=c_{2}-y * A_{1}\right.  \tag{3.74}\\
\text { in } \left.s_{2}^{+} * u^{+}+s_{1}^{+} * u^{-}+s_{2}^{-} * l^{+}+s_{1}^{-} * l^{-}\right) .
\end{gather*}
$$

is just what we need and is because of $y_{1} \geq 0$ a direct consequence of 3.72 . To validate that this is the theorem we are looking for, we need to assure ourselves that

$$
\begin{equation*}
c-y * A \approx 0 \tag{3.75}
\end{equation*}
$$

holds. Because $y^{\prime}$ is a certificate for the modified linear program we have

$$
0 \approx c^{\prime}-y^{\prime} * A^{\prime}=\left(\begin{array}{ll}
c & K
\end{array}\right)-\left(\begin{array}{lll}
y & y_{1} & y_{2}
\end{array}\right) *\left(\begin{array}{cc}
A & b \\
0 & 1 \\
0 & -1
\end{array}\right)=\left(\begin{array}{ll}
c-y * A \quad K-\left(y * b+y_{1}-y_{2}\right)
\end{array}\right)
$$

Focusing on the first component in the above confirms (3.75), and therefore also the usefulness of (3.74).

We know now how to prove any bound we desire for any objective function $c * x$ of the original infeasible linear program. Actually, we get a particularly nice objective function by choosing $c=0$. Specializing theorem (3.74) to $c=0$ results in:

$$
\begin{align*}
& \llbracket A * x \leq b ; A_{1} \leq A ; A \leq A_{2} ; l \leq x ; x \leq u ; 0 \leq y ; 0 \leq y_{1} \rrbracket \\
& \Longrightarrow 0 \leq y * b+y_{1}+\left(\operatorname{let} s_{1}=-y * A_{2} ; s_{2}=-y * A_{1}\right.  \tag{3.76}\\
& \left.\quad \text { in } s_{2}^{+} * u^{+}+s_{1}^{+} * u^{-}+s_{2}^{-} * l^{+}+s_{1}^{-} * l^{-}\right) .
\end{align*}
$$

Choosing a modification parameter $K$ such that $K<0$, for example $K=-1$, calculating a certificate $y, y_{1}$ for this modified LP, plugging this certificate into (3.76), and computing it will lead to the following theorem:

$$
\begin{align*}
& \llbracket \boldsymbol{A} * \boldsymbol{x} \leq b ; A_{1} \leq \boldsymbol{A} ; \boldsymbol{A} \leq A_{2} ; l \leq \boldsymbol{x} ; \boldsymbol{x} \leq u \rrbracket  \tag{3.77}\\
& \Longrightarrow \text { False }
\end{align*}
$$

We have arrived at an Isabelle theorem expressing the infeasibility of the original linear program. Free variables of the theorem are set in bold face again.

### 3.6 Sparse Matrices

After reading the previous sections, you probably wonder what a matrix numeral might look like. We have chosen to represent matrix numerals in such a way that sparse matrices are encoded efficiently:

```
types
    \alpha spvec = (nat * \alpha) list
    \alpha spmat = (\alpha spvec) spvec
constdefs
    sparse-row-vector :: \alpha spvec }=>\alpha\mathrm{ matrix
    sparse-row-vector l \equiv foldl( }\lambdam(i,e).m+(\mathrm{ singleton-matrix0ie))0l
    sparse-row-matrix :: }\alpha\mathrm{ spmat }=>\alpha\mathrm{ matrix
    sparse-row-matrix L \equiv
        foldl(\lambdam(j,l).m+(move-matrix(sparse-row-vectorl) j0)) 0L
```

Here singleton-matrix jie denotes the matrix whose elements are all zero except the element in row $j$ and column $i$, which equals $e$. Furthermore move-matrix $A j i$ denotes the matrix that one gets if one moves the matrix $A$ by $j$ rows down and $i$ columns right, and fills up the first $j$ rows and $i$ columns with zero elements.

Here is an example of a matrix numeral:

$$
\begin{aligned}
& {[(1,[(1,7),(3,13)]),(2,[(0,-4),(1,47)])]} \\
& \xrightarrow{\text { sparse-row-matrix }}\left(\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 7 & 0 & 13 \\
-4 & 47 & 0 & 0
\end{array}\right)
\end{aligned}
$$

We have formalized addition, subtraction, multiplication, comparison, positive part and negative part directly on sparse vectors and matrices by recursion on lists. The multiplication algorithm for sparse matrices is inspired by the one given in [10].

These operations on sparse vectors/matrices can be proven correct with respect to their finite matrices counterpart via the sparse-row-matrix morphism, assuming certain sortedness constraints. This is actually not too hard: all students of an introductory Isabelle/HOL class taught at Technische Universität München have been able to complete these proofs within four weeks as their final assignment with varying help from their tutors. Using these correctness results, one can then easily prove a sparse version of (3.72).

### 3.7 Interval Arithmetic

### 3.7.1 Floats

Real numbers are represented as binary, arbitrary precision floating point numbers:

```
constdef
    float :: (int* int) }=>\mathrm{ real
    float }(m,e)\equiv(\mathrm{ real m)* 2e
```

In the above, $m$ is called the mantissa, and $e$ the exponent. The Isabelle theorem

```
float (a, , e })+\mathrm{ float ( }\mp@subsup{a}{2}{},\mp@subsup{e}{2}{})
    if e}\mp@subsup{e}{1}{}\leq\mp@subsup{e}{2}{}\mathrm{ then float (a}+\mp@subsup{a}{2}{}*\mp@subsup{a}{}{\wedge}\mp@subsup{}{}{\wedge}\mathrm{ nat (e}\mp@subsup{e}{2}{}-\mp@subsup{e}{1}{}),\mp@subsup{e}{1}{}
    else float ( }\mp@subsup{a}{1}{* 2 ^ nat (e. ( - e2) + a 2, e}2
```

shows how to perform addition in this representation, multiplication is even easier:

$$
\begin{equation*}
\text { float }\left(a_{1}, e_{1}\right) * \text { float }\left(a_{2}, e_{2}\right)=\text { float }\left(a_{1} * a_{2}, e_{1}+e_{2}\right) \tag{3.82}
\end{equation*}
$$

We prefer a floating point representation over a representation by fractions because addition of floating point numbers is cheaper and easier to perform than addition of fractions. We will often want to multiply matrices with real numbers as entries, and there addition and multiplication of real numbers are the dominant operations.

Other operations like the positive and the negative part are also easily definable for floats. Division is problematic, though. Take for example the real number expressed by the fraction $\frac{1}{3}$. There are no $m, e$ such that float $(m, e)=\frac{1}{3}$. But because our floating point representation is arbitrary precision, it is of course no problem to approximate $\frac{1}{3}$ by floats as precise as we wish for. E.g., up to a precision of $2^{-50}$ :

```
float (375299968947541,-50) \(\leq \frac{1}{3} \leq\) float (750599937895083,-51)
```

The failure of floats to represent certain fractions directly is no reason to abandon the float representation and to prefer fractions instead. When we later turn to the basic linear programs we will have to compute with values like $\pi$ or $\sqrt{2}$ which even fractions cannot represent directly, therefore approximation is inevitable.

We want to develop algorithms for floats, e.g. division, and we want these algorithms to be functions within the logic, so that we can apply the HOL Computing Library to it. These algorithms need to be able to break a float into its components mantissa and exponent. Because float $(m, e)$ is just a real number, and there are no such things as the mantissa and exponent of a real number, we need to introduce a new type of floats.

```
datatype float = Float int int
fun Ifloat :: float }=>\mathrm{ real
where
Ifloat (Float a b) = float (a,b)
```

Operations like addition, multiplication and so on can be defined on this type. All of these operations must commute with the Ifloat morphism. One can show that the type float is an instance of the axiomatic type class of commutative semirings. It is not the case that float is an instance of the type class order, because then it would have to fulfill $(x<y)=(x \leq y \wedge x \neq y)$ which is clearly not the case.

### 3.7.2 Division of Floats

We approach the division algorithm in four steps. We first approximate nonnegative true fractions like $\frac{1}{3}$ or $\frac{4}{5}$. We then move on to approximating any nonnegative fraction, like $\frac{10}{7}$, and finally to approximating any fraction, including negative ones. From there it is straightforward to define division of floats.

The lapprox-frac and the rapprox-frac functions approximate a nonnegative true fraction from the left and the right, respectively. The quality of the approximation can be controlled by a counter that determines the number of approximation steps. By a flag one can stop this counter from counting until the significant digits of the number have been reached.

```
function lapprox-frac :: bool \(\Rightarrow\) nat \(\Rightarrow\) int \(\Rightarrow\) int \(\Rightarrow\) float
where
    lapprox-frac flag \(0 \times y=0\)
\(\mid x \leq 0 \Longrightarrow\) lapprox-frac flag \(n x y=0\)
| \(0<x \Longrightarrow 0<n \Longrightarrow\)
    lapprox-frac flag \(n x y=\)
        (if \(2 * x \geq y\) then Float \(1-1+\) Float \(1-1 *\) lapprox-frac True \((n-1)(2 * x-y) y\)
        else Float \(1-1 *\) lapprox-frac flag (if flag then \((n-1)\) else \(n)(2 * x) y\) )
    function rapprox-frac :: bool \(\Rightarrow\) nat \(\Rightarrow\) int \(\Rightarrow\) int \(\Rightarrow\) float
    where
        rapprox-frac flag \(0 x y=(\) if \(x \leq 0\) then 0 else 1\()\)
        \(\mid x \leq 0 \Longrightarrow\) rapprox-frac flag \(n x y=0\)
\(\mid 0<x \Longrightarrow 0<n \Longrightarrow\)
        rapprox-frac flag \(n x y=\)
        (if \(2 * x \geq y\) then Float \(1-1+\) Float \(1-1 *\) rapprox-frac True \((n-1)(2 * x-y)\) y
        else Float \(1-1 *\) rapprox-frac flag (if flag then \((n-1)\) else \(n)(2 * x) y\) )
```

In order to define these functions one has to prove termination, which was surprisingly difficult, involving over 150 lines of proof.

The correctness of lapprox-frac and rapprox-frac is stated in (3.86) and (3.87).

$$
\begin{align*}
& 0 \leq x \Longrightarrow x<y \Longrightarrow \\
& 0 \leq \text { Ifloat (lapprox-frac flag } n x y \text { ) }  \tag{3.86}\\
& \wedge \text { Ifloat (lapprox-frac flag } n x y \text { ) } \leq \text { real } x / \text { real } y \\
& 0 \leq x \Longrightarrow x<y \Longrightarrow \text { real } x / \text { real } y \leq \text { Ifloat (rapprox-frac flag } n x y \text { ) } \tag{3.87}
\end{align*}
$$

Note that we did not prove any theorems about the quality of the approximation, which are not needed for our formal development, but tests show it to be as expected. We will now deal with any nonnegative fraction:

```
definition lapprox-posrat :: nat \(\Rightarrow\) int \(\Rightarrow\) int \(\Rightarrow\) float
where
    lapprox-posrat prec \(x y=\)
    (let
        \(d=x \operatorname{div} y ;\)
        \(m=x \bmod y\)
    in
        Float \(d 0+\) lapprox-frac \((d \neq 0)(\) prec - nat \((\) bitlen \(d)) m y)\)
definition rapprox-posrat :: nat \(\Rightarrow\) int \(\Rightarrow\) int \(\Rightarrow\) float
where
    rapprox-posrat prec \(x\) y \(=\)
    (let
        \(d=x \operatorname{div} y ;\)
        \(m=x \bmod y\)
    in
        Float \(d 0+\) rapprox-frac \((d \neq 0)(\) prec - nat \((\) bitlen \(d)) m y)\)
```

The function bitlen counts the number of bits of its argument. The correctness results for lapprox-posrat and rapprox-posrat are similar to (3.86) and (3.87), but with the condition $x<y$ weakened to $0<y$.

Approximating any fraction is now just a matter of case distinction:

```
function lapprox-rat :: nat \(\Rightarrow\) int \(\Rightarrow\) int \(\Rightarrow\) float
where
    \(y=0 \Longrightarrow\) lapprox-rat prec \(x y=0\)
\(\mid 0 \leq x \Longrightarrow 0<y \Longrightarrow\) lapprox-rat prec \(x y=\) lapprox-posrat prec \(x y\)
\(\mid x<0 \Longrightarrow 0<y \Longrightarrow\) lapprox-rat prec \(x y=-\) (rapprox-posrat prec ( \(-x\) ) y)
\(\mid x<0 \Longrightarrow y<0 \Longrightarrow\) lapprox-rat prec \(x y=\) lapprox-posrat prec \((-x)(-y)\)
\(\mid 0 \leq x \Longrightarrow y<0 \Longrightarrow\) lapprox-rat prec \(x y=-(\) rapprox-posrat prec \(x(-y)\) )
function rapprox-rat :: nat \(\Rightarrow\) int \(\Rightarrow\) int \(\Rightarrow\) float
where
    \(y=0 \Longrightarrow\) rapprox-rat prec \(x y=0\)
\(\mid 0 \leq x \Longrightarrow 0<y \Longrightarrow\) rapprox-rat prec \(x y=\) rapprox-posrat prec \(x\) y
\(\mid x<0 \Longrightarrow 0<y \Longrightarrow\) rapprox-rat prec \(x y=-\) (lapprox-posrat prec ( \(-x\) ) y)
\(\mid x<0 \Longrightarrow y<0 \Longrightarrow\) rapprox-rat prec \(x y=\) rapprox-posrat prec \((-x)(-y)\)
\(\mid 0 \leq x \Longrightarrow y<0 \Longrightarrow\) rapprox-rat prec \(x y=-\) (lapprox-posrat prec \(x(-y)\) )
```

Here are the theorems about the correctness of these functions:

$$
\begin{equation*}
\text { Ifloat (lapprox-rat prec } x \text { y) } \leq \text { real } x / \text { real } y \tag{3.92}
\end{equation*}
$$

$$
\begin{equation*}
\text { real x / real } y \leq \text { Ifloat (rapprox-rat prec } x \text { y) } \tag{3.93}
\end{equation*}
$$

Finally, we can compute the division of floats:

```
fun float-divl :: nat \(\Rightarrow\) float \(\Rightarrow\) float \(\Rightarrow\) float
where
    float-divl prec \(\left(\right.\) Float \(\left.m_{1} s_{1}\right)\left(\right.\) Float \(\left.m_{2} s_{2}\right)=\)
        (let
        1 = lapprox-rat prec \(m_{1} m_{2}\);
        \(f=\) Float \(1\left(s_{1}-s_{2}\right)\)
        in
        \(f * 1)\)
fun float-divr :: nat \(\Rightarrow\) float \(\Rightarrow\) float \(\Rightarrow\) float
where
    float-divr prec \(\left(\right.\) Float \(\left.m_{1} s_{1}\right)\left(\right.\) Float \(\left.m_{2} s_{2}\right)=\)
    (let
        \(r\) = rapprox-rat prec \(m_{1} m_{2}\);
        \(f=\) Float \(1\left(s_{1}-s_{2}\right)\)
    in
        \(f * r)\)
```

The correctness is an immediate corollary of (3.92) and (3.93), respectively:

```
Ifloat (float-divl prec x y) \leq Ifloat x / Ifloat y
Ifloat x / Ifloat y \leq Ifloat (float-divr prec x y)
```


### 3.7.3 Basic Interval Arithmetic for Floats

We have seen how to formalize addition, multiplication and division for floats. Addition and multiplication commute with the Ifloat morphism; by that we mean that the formulas

$$
\begin{equation*}
\text { Ifloat }(u+v)=\text { Ifloat } u+\text { Ifloat } v, \quad \text { Ifloat }(u * v)=\text { Ifloat } u * \text { Ifloat } v \tag{3.98}
\end{equation*}
$$

are true for all $u, v$ of type float. As we have seen, this is not true for division; there is no function $d$ on floats with the property

$$
\begin{equation*}
\text { Ifloat }(d u v)=\text { Ifloat } u / \text { Ifloat } v \tag{3.99}
\end{equation*}
$$

for all $u, v$ of type float. Also, we might be interested in different addition and multiplication operations than those exact ones with the commute property. E.g., imagine that throughout a computation we do not want to use more than 30 binary digits.

The commute property is especially nice when evaluating larger expressions which consist of nested elementary operations. Let's say we have four real numbers $x_{1}, x_{2}, x_{3}, x_{4}$ together with their float representations $x_{i}=$ Ifloat $r_{i}$. Then calculating $x_{1}+\left(x_{2} *\left(x_{3}+x_{4}\right)\right)$ is just a matter of simple rewriting:

$$
\begin{align*}
x_{1}+\left(x_{2} *\left(x_{3}+x_{4}\right)\right) & =\text { Ifloat } r_{1}+\left(\text { Ifloat } r_{2} *\left(\text { Ifloat } r_{3}+\text { Ifloat } r_{4}\right)\right. \\
& =\text { Ifloat }\left(r_{1}+\left(r_{2} *\left(r_{3}+r_{4}\right)\right)\right)  \tag{3.100}\\
& =\text { float }(a, b)
\end{align*}
$$

where $r_{1}+\left(r_{2} *\left(r_{3}+r_{4}\right)\right)$ rewrites to Float $a b$.

Losing the commute property means losing this simple way of evaluating nested operations by rewriting, because now the relationship between two steps in the computation is not equality any more, but something more complicated.

We do not want to give up the speed of rewriting with the HOL Computing Library; fortunately, there is a solution to our problem. We introduce a new datatype which represents nested expressions of basic operations:

```
datatype basicarith =
    Plus basicarith basicarith | Sub basicarith basicarith | Minus basicarith
| Mult basicarith basicarith | Div basicarith basicarith | Inverse basicarith
| Atom nat | Num float
```

The Atom constructor acts as a variable in de-Bruijn representation, so that atomic values which do not correspond to any other basicarith constructor can nevertheless be incorporated into the expression. In order to assign meaning to a basicarith expression we need to bind those variables to values. Therefore the Ibasicarith function not only takes a basicarith term as an argument, but also an environment of real numbers which is supposed to bind any variable occurring in the term.

```
fun Ibasicarith :: real list \(\Rightarrow\) basicarith \(\Rightarrow\) real
where
    Ibasicarith vs (Plus a b) \(=(\) Ibasicarith vs a) \(+(\) Ibasicarith vs \(b)\)
    \(\mid\) Ibasicarith vs \((\) Sub a b) \()=(\) Ibasicarith vs a) \(-(\) Ibasicarith vs \(b)\)
\(\mid\) Ibasicarith vs (Minus a) \(=-(\) Ibasicarith vs a)
\(\mid\) Ibasicarith vs (Mult a b) \(=(\) Ibasicarith vs a) \(*(\) Ibasicarith vs \(b)\)
| Ibasicarith vs (Div a b) \(=(\) Ibasicarith vs a) / (Ibasicarith vs b)
| Ibasicarith vs (Inverse a) \(=1\) / (Ibasicarith vs a)
| Ibasicarith vs \((\) Num \(f)=\) Ifloat \(f\)
| Ibasicarith vs \((\) Atom \(n)=v s!n\)
```

The expression vs! $n$ picks the $n$-th element out of the list vs.
One can understand the basicarith type as an extension of the float type such that every operation on the real numbers we are interested in has a corresponding commuting operation.

How do we use the Ibasicarith morphism for evaluating nested expressions? Look at the expression

$$
\frac{\pi+4}{\sqrt{2}}
$$

There are two values in this expression, $\pi$ and $\sqrt{2}$, which cannot be represented directly as basicarith terms. We factor them out and turn them into variables. This gives us:

$$
\begin{equation*}
\frac{\pi+4}{\sqrt{2}}=I \text { basicarith }[\pi, \sqrt{2}](\operatorname{Div}(\text { Add }(\text { Atom } 0)(\text { Num }(\text { Float } 12)))(\text { Atom } 1)) . \tag{3.103}
\end{equation*}
$$

We want to approximate the right hand side using interval arithmetic. We define
an approximation function on basicarith:

```
function approx :: nat \(\Rightarrow\) (float \(*\) float) list \(\Rightarrow\) basicarith \(\Rightarrow\) (float \(*\) float) option
where
    approx \(n\) bs (Atom i) \(=(\) if \(i<\) length bs then Some (bs \(!i)\) else None \()\)
\(\mid\) approx \(n\) bs \((\operatorname{Num} f)=\) Some \((f, f)\)
\(\mid\) approx \(n\) bs (Plus a \(b\) ) \(=\)
    lift-bin (approx \(n\) bs a) (approx \(n b s b\) )
    \(\left(\lambda a_{1} a_{2} b_{1} b_{2}\right.\). Some \(\left.\left(a_{1}+b_{1}, a_{2}+b_{2}\right)\right)\)
\(\mid\) approx \(n\) bs \((\) Sub ab) \()=\)
    lift-bin (approx \(n\) bs a) (approx \(n\) bs b)
    \(\left(\lambda a_{1} a_{2} b_{1} b_{2}\right.\). Some \(\left.\left(a_{1}-b_{2}, a_{2}-b_{1}\right)\right)\)
\(\mid \operatorname{approx} n\) bs (Multa \(b)=\)
    lift-bin (approx \(n\) bs a) (approx \(n b s b)\)
    ( \(\lambda a_{1} a_{2} b_{1} b_{2}\). Some
            (float-nprt \(a_{1} *\) float-pprt \(b_{2}+\) float-nprt \(a_{2} *\) float-nprt \(b_{2}\)
        + float-pprt \(a_{1} *\) float-pprt \(b_{1}+\) float-pprt \(a_{2} *\) float-nprt \(b_{1}\),
        float-pprt \(a_{2} *\) float-pprt \(b_{2}+\) float-pprt \(a_{1} *\) float-nprt \(b_{2}\)
        + float-nprt \(a_{2} *\) float-pprt \(b_{1}+\) float-nprt \(a_{1} *\) float-nprt \(\left.b_{1}\right)\) )
\(\mid \operatorname{approx} n b s(\) Inverse \(a)=\)
    lift-un (approx \(n\) bs a)
        ( \(\lambda a_{1} a_{2}\). if \(\left(0<a_{1} \vee a_{2}<0\right)\) then
                        Some (float-divl n \(1 a_{2}\), float-divr n \(1 a_{1}\) )
                    else None)
\(\mid\) approx \(n\) bs (Div a b) \(=\) approx \(n\) bs (Mult a (Inverse b))
\(\mid\) approx \(n\) bs (Minus a) \(=\) lift-un (approx \(n\) bs a) \(\left(\lambda a_{1} a_{2}\right.\). Some \(\left.\left(-a_{2},-a_{1}\right)\right)\)
```

Given an environment $b s$ that consists of intervals of floats for each bound variable, approx prec bs $t$ will return an interval of floats that approximates $t$. It might not be able to compute such an interval; then it returns indicating a failure. If the term makes no use of division or inversion, the returned interval will be the tightest one possible. Use of division or inversion introduces approximation; the quality of this approximation is controlled by the prec parameter. The algorithm should be fairly self-explaining. Because each recursive call to approx may fail (inversion of an interval containing 0 is not possible), we use functions lift-un(ary) and lift-bin(ary) which either propagate the failure, or continue processing in case of success. We deal with the case for multiplication using our formula for estimating a product by the positive and negative part of its components (3.71). Division is delegated to inversion, and inversion is dealt with using the algorithms for division of floats from Section 3.7.2.

To express the correctness of approx we need to define a predicate which says if a list of real numbers is bounded by a list of intervals:

$$
\begin{align*}
& \text { definition } \\
& \text { bounded-by :: real list } \Rightarrow(\text { float } * \text { float }) \text { list } \Rightarrow \text { bool } \\
& \text { where }  \tag{3.105}\\
& \text { bounded-by vs bs }= \\
& \quad(\forall i . i<\text { length bs } \longrightarrow \operatorname{Ifloat~}(\text { fst }(\text { bs }!i)) \leq \text { vs }!i \wedge \text { vs }!i \leq \text { Ifloat }(\text { snd }(b s!i)))
\end{align*}
$$

The correctness result for approx can then be stated like this:
$\llbracket$ bounded-by vs bs; approx prec bs expr $=$ Some $(1, r) \rrbracket \Longrightarrow$
Ifloat $1 \leq$ Ibasicarith vs expr $\wedge$ Ibasicarith vs expr $\leq$ Ifloat $r$

Let us finish the example we started in (3.103). We turn bounds for $\pi$ and $\sqrt{2}$

$$
\begin{equation*}
\text { bounded-by }[\pi, \sqrt{2}][(\text { Float } 30 \text {, Float } 12),(\text { Float } 10, \text { Float } 11)] \tag{3.107}
\end{equation*}
$$

into an approximation of $(\pi+4) / \sqrt{2}$ :

$$
\begin{align*}
& \text { approx } 1[(\text { Float } 3 \text { 0, Float } 1 \text { 2),(Float } 1 \text { 0, Float } 1 \text { 1)] } \\
& \begin{array}{l}
(\text { Div }(\text { Add (Atom 0)(Num (Float } 12))) \\
=\text { Some }(\text { Float } 7-1, \text { Float } 13)
\end{array} \tag{3.108}
\end{align*}
$$

Plugging (3.107) and (3.108) into (3.106) and applying (3.103) yields the theorem

$$
\begin{equation*}
\text { float }(7,-1) \leq \frac{\pi+4}{\sqrt{2}} \quad \wedge \quad \frac{\pi+4}{\sqrt{2}} \leq \text { float }(1,3) \tag{3.109}
\end{equation*}
$$

### 3.7.4 Approximation of Matrices

Let us assume that the matrix $A$ of a linear program is given by a matrix with elements like $\frac{\pi+4}{\sqrt{2}}$. We know how to approximate a single element of this matrix; in order to apply our methods for bounding linear programs, we need to approximate all entries of the matrix and obtain both a lower bound $A_{1}$ and an upper bound $A_{2}$ for $A$. We achieve this by lifting approx to the level of matrices. The signature for a version of approx for sparse matrices is:

$$
\begin{align*}
& \text { approx-spmat }:: \\
& \text { nat } \Rightarrow \text { (float } * \text { float }) \text { list } \Rightarrow \text { basicarith spmat } \Rightarrow \text { (float spmat } * \text { float spmat }) \text { option. } \tag{3.110}
\end{align*}
$$

In our application there are many entries of the matrix which are equal. Therefore factoring out whole equal entries as variables and approximating them separately significantly improves the performance of the approximation.

### 3.8 Calculating A Priori Bounds

Both the method of proving bounds for feasible linear programs from Section 3.4 and the method of proving infeasibility from Section 3.5 require a priori knowledge of bounds for the vector $x$. We might be able to read particularly obvious bounds off the constraints $A * x \leq b$. Consider for example the case that one row

$$
a_{j}=\left(\begin{array}{lll}
a_{j, 1} & \ldots & a_{j, n}
\end{array}\right) \quad \text { of } \quad A=\left(\begin{array}{c}
a_{1} \\
\vdots \\
a_{m}
\end{array}\right)
$$

has only one non-null entry, say $a_{j, i}$. Then either $x_{i} \leq b_{j} / a_{j, i}$ if $a_{j, i}>0$ or $x_{i} \geq b_{j} / a_{j, i}$ if $a_{j, i}<0$.
There are more easy cases we can handle. Let us again single out the matrix entry $a_{j, i} \neq 0$ but this time we do not necessarily assume all other entries in the same row to be zero. We know $\sum_{k=1}^{n} a_{j, k} x_{k} \leq b_{j}$, or, after moving all terms except $a_{j, i} x_{i}$ to the right hand side of the inequality,

$$
\begin{equation*}
a_{j, i} x_{i} \leq b_{j}+\sum_{k \in\{1, \ldots, n\}, k \neq i}\left(-a_{j, k} x_{k}\right) . \tag{3.111}
\end{equation*}
$$

The term $-a_{j, k} x_{k}$ can be bounded from the above in one of these cases:

- $a_{j, k}=0$,
- $a_{j, k}>0$, and we already know a lower bound for $x_{k}$,
- $a_{j, k}<0$, and we already know an upper bound for $x_{k}$.

If we can thus bound for all $k \neq i$ the terms $-a_{j, k} x_{k}$ then we can bound $x_{i}$ from above if $a_{j, i}>0$, or we can bound $x_{i}$ from below if $a_{j, i}<0$.

We repeat adding such easy bounds to our list of known bounds for $x$ until the set of indices $i$ for which we know a lower bound of $x_{i}$ and the set of indices $i$ for which we know an upper bound of $x_{i}$ do not change any more. This computation is performed outside the logic. What we have got after finishing the computation is a certificate for proving formally within the logic bounds for the components of $x$. This certificate is just a list of triples ( $j, i, k s$ ), where $i$ denotes the row $x_{i}$ we are going to bound, $j$ denotes the row $a_{j}$ and $k s$ is the set of indices $k \neq i$ such that $a_{j, k} \neq 0$.

We work the certificate from its first to its last element. For a single element of the certificate we instantiate the following theorem:

```
\(\llbracket A_{1} \leq A ; A \leq A_{2} ; A * x \leq b ;\)
    row-of-matrix \(A_{1} j=a_{1}\); row-of-matrix \(A_{2} j=a_{2}\);
    nullify-column \(a_{1} i=u_{1}\); nullify-column \(a_{2} i=u_{2}\);
    filter-cols \(u_{1} k s=u_{1}\); filter-cols \(u_{2} k s=u_{2}\);
    filter-rows \(x\) ks \(=x^{\prime} ; x_{1} \leq x^{\prime} ; x^{\prime} \leq x_{2}\);
    Rep-matrix \(a_{1} 0 i=\) float \(\left(m_{1}, e_{1}\right) ;\) Rep-matrix \(a_{2} 0 i=\) float \(\left(m_{2}, e_{2}\right)\);
    Rep-matrix b j 0 - Rep-matrix ( \(u_{1}^{-} * x_{2}^{+}+u_{2}^{-} * x_{2}^{-}+u_{1}^{+} * x_{1}^{+}+u_{2}^{+} * x_{1}^{-}\)) \(00=\) float ( \(m, e\) );
    approx prec \(\left[\left(\right.\right.\) Float \(m_{1} e_{1}\), Float \(\left.\left.m_{2} e_{2}\right)\right]\) (Div (Num (Float me)) \()^{2}(\) Atom 0)) \(=\) Some (lapprox, rapprox) 】
\(\Longrightarrow\) if \(0<m_{1}\) then Rep-matrix x \(0 \leq\) Ifloat rapprox
    else if \(m_{2}<0\) then Ifloat lapprox \(\leq\) Rep-matrix xi 0
    else True
```

The first line of (3.112) sets the context; we have a system of linear inequalities $A * x \leq b$, and the matrix $A$ is approximated by matrices $A_{1}$ and $A_{2}$. The rest of the theorem can be read like a program with occasional assertions. We calculate the $j$-th row of $A_{1}$ and $A_{2}$ and store them in $a_{1}$ and $a_{2}$, respectively. Then the $i$-th column of $a_{1}$ and $a_{2}$ are set to 0 , resulting in $u_{1}$ and $u_{2}$. Next we need to ensure that the set $k s$ really contains all indices $k$ for which the $k$-th column of $a_{j}$ is non-zero. This is what filter-cols $u_{1} k s=u_{1}$ and filter-cols $u_{2} k s=u_{2}$ check; if we retrieve all columns of $u_{1}$ with indices in $k s$ by setting all other columns to 0 , and the result is $u_{1}$, then clearly setting the other columns to 0 has not changed anything, so they must have been 0 before. The same holds for $u_{2}$. The next line of the program, filter-rows $x k s=x^{\prime}$, acknowledges the fact that only those rows of $x$ with indices in $k s$ are relevant for calculating the bound. We check then that these rows can be bounded by $x_{1}$ and $x_{2}$, where $x_{1}$ and $x_{2}$ have been obtained by the previous steps of working the certificate.

Next we store the lower and the upper bound for $a_{j, i}$ as float $\left(m_{1}, e_{1}\right)$ and float $\left(m_{2}, e_{2}\right)$. We then calculate an upper bound of the right hand side of Equation 3.111 and store the result as float $(m, e)$. Dividing float $(m, e)$ by $a_{j, i}$ gives us an upper bound for $x_{i}$ if $a_{j, i}>0$, and a lower bound if $a_{j, i}<0$.

It would be nice if our theorem prover could understand (3.112) as a program with assertions as we just explained it. The HOL Computing Library allows the theorem prover to see them that way. In Section 2.6 .4 we outlined the HCL's capabilities of mixing modus ponens, variable instantiation and computing. This is what is needed here. We first internalize Theorem (3.112) as HCL theorem and use modus ponens to discharge the first three assumptions, thereby setting the context. This gives us an HCL theorem $\Psi$. For each element $e=(j, i, k s)$ of the certificate we then instantiate the corresponding variables in $\Psi$, resulting in an HCL theorem $\Psi_{e}$. Eliminating all assumptions of $\Psi_{e}$ and exporting the result gives us an Isabelle theorem that states a bound for $x_{i}$.

Finally, note that actually we do not use 3.112 directly but a version for sparse matrices derived from it.

## CHAPTER 4

## The Basic Linear Programs

> Reality is that which, when you stop believing in it, doesn't go away.
> — Philip K. Dick

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### 4.1 The Archive Of Tame Graphs

The result of the first major completed part of the Flyspeck project is the verification of an archive of tame graphs [23]. Tame graphs are special planar graphs that represent possible counterexamples to the Kepler conjecture. There are only finitely many, and that is why it is possible to have an archive of all of them.

There are various ways of representing and formalizing planar graphs [3]. As a planar graph consists of nodes, edges and faces, one possibility to represent a planar graph would be a list of faces, where each face is again a list of nodes, leaving the representation of the edges implicit in the arrangement of nodes. This is the representation used in [23].

For our work we choose to represent planar graphs by hypermaps. Hypermaps have been introduced to mechanized theorem proving by Gonthier in his proof of the Four Color Theorem [8]. It builds on the notion of dart. Darts can be viewed as the oriented edges of a graph (Gonthier chooses a different, but equivalent, point of view; he sees them as angles between incident edges of the same face). Let us assume that we are given three permutations $e, n$ and $f$ of a finite set $D$ of darts. Two darts $\alpha$ and $\beta$ are called equivalent with respect to a permutation $p$ of $D$ iff $\exists n . \alpha=p^{n} \beta$ holds. The such induced relation on darts is an equivalence relation, and we write $|p|$ for its number of equivalence classes. If now the given three permutations fulfill
the equations

$$
\begin{equation*}
e=e^{-1}=n \circ f \quad \text { and } \quad 2|e|=|D| \quad \text { and } \quad|e|+|f|+|n|=|D|+2, \tag{4.1}
\end{equation*}
$$

then we can construct a connected planar graph in the following way:

1. The nodes, edges and faces are the equivalence classes of $n, e$ and $f$.
2. An edge $E=\left\{\delta_{1}, \delta_{2}\right\}$ consists therefore of the two oriented edges $\delta_{1}$ and $\delta_{2}$.
3. There is an oriented edge $\delta$ from node $N_{1}$ to node $N_{2}$ iff $\delta \in N_{1}$ and $e \delta \in N_{2}$.
4. An oriented edge $\delta$ belongs to a face $F$ iff $\delta \in F$.

Figure 4.1: A planar graph


Consider the planar graph in Fig. 4.1. Each dart is denoted by a number, and we have $D=\{0,1,2, \ldots, 11\}$. The permutations are given by

$$
\begin{align*}
& f=(0 \mapsto 1 \mapsto 2 \mapsto 3 \mapsto 4,5 \mapsto 6 \mapsto 7,8 \mapsto 9 \mapsto 10 \mapsto 11), \\
& e=(0 \mapsto 11,1 \mapsto 10,2 \mapsto 9,3 \mapsto 6,4 \mapsto 5,7 \mapsto 8)  \tag{4.2}\\
& n=(0 \mapsto 5 \mapsto 8,1 \mapsto 11,2 \mapsto 10,3 \mapsto 9 \mapsto 7,4 \mapsto 6) .
\end{align*}
$$

It might be instructive to check the equations (4.1).
Darts are also viewed as faces, nodes and edges. For example, there are three faces, face 0 , face 5 , and face 8 (to see why there are three faces, not two, imagine how the graph looks when drawn on a sphere instead of in the plane); and face 7 is the same as face 5 .

We have converted the archive of tame graphs [22] into the hypermap representation and formalized them as values of type (nat $\times$ nat $\times$ nat) NatTreeMap where

$$
\begin{equation*}
\text { datatype } \alpha \text { NatTreeMap }=\operatorname{TIN} \text { nat } \alpha(\alpha \text { NatTreeMap) }(\alpha \text { NatTreeMap) } \mid T N N \tag{4.3}
\end{equation*}
$$

An $\alpha$ NatTreeMap represents a function via the eval function:

```
fun eval \(:: \alpha\) NatTreeMap \(\Rightarrow\) nat \(\Rightarrow \alpha\) option
where
    eval TNN \(x=\) None
| eval (TIN \(x\) cab) \(x^{\prime}=\)
        if \(x=x^{\prime}\) then Some \(c\) else if \(x^{\prime}<x\) then eval a \(x^{\prime}\) else eval \(b x^{\prime}\)
```

The face, edge, and node permutations of a graph represented as value of type (nat $\times$ nat $\times$ nat) NatTreeMap can therefore be accessed through the following three functions:

```
constdefs
    map-face :: (nat }\times\mathrm{ nat }\times\mathrm{ nat) NatTreeMap }=>\mathrm{ nat }=>\mathrm{ nat
    map-face m d = fst (the (eval m d))
    map-edge :: (nat }\times\mathrm{ nat }\times\mathrm{ nat) NatTreeMap }=>\mathrm{ nat }=>\mathrm{ nat
    map-edge m d = fst (snd (the (eval m d)))
    map-node :: (nat }\times\mathrm{ nat }\times\mathrm{ nat) NatTreeMap }=>\mathrm{ nat }=>\mathrm{ nat
    map-node m d = snd (snd (the (eval m d)))
```

The complete archive of 2771 tame graphs is given in our formalization as a constant Archive of type (nat $\times$ nat $\times$ nat) NatTreeMap list, each element of the list representing a tame graph. For convenience, there are also 2771 constants
graph-1, ..., graph-2771
of type (nat $\times$ nat $\times$ nat) NatTreeMap, each constant representing a tame graph.

### 4.2 Graph Systems

A graph system models a planar graph together with

- a fixed set of variables defined on the darts of the planar graphs,
- constraints relating these variables.

In [16, sec. 23.3] Hales sketches what he calls the basic linear programs. Our notion of graph system is intended to encompass those basic linear programs and give a complete specification of them. It does not capture the more complicated linear programs which result from branch-and-bound methods. In order to handle those linear programs, it would be necessary to add more variables to the graph system and to change the constraints on them.

Note that a graph system is a way to ascribe certain properties to a given planar graph. We do not intend the graph system to model the notion of planarity exactly; for example, we do not require the graph induced by a graph system to fulfill all of the properties in (4.1). But for the concrete instances of graph systems we are dealing with these equations will hold, of course, because these concrete instances are based on tame graphs, and tame graphs are planar.

We manage the data of a graph system as a record of type $\alpha G S$. The type parameter $\alpha$ denotes the type of darts. We require that there is a linear order defined on $\alpha$. As in our application $\alpha$ will always be nat, this is not a problem.

There are two kinds of record components: those members which describe the topology of the planar graph (fig. 4.2), and those members which represent the variables on darts (fig. 4.3); all variables have values in $\mathbb{R}$. Note that although e.g. the type of $g s-\sigma$ is stated to be $\alpha \Rightarrow$ real, it really is $\alpha G S \Rightarrow \alpha \Rightarrow$ real, taking an explicit graph system record as parameter.

What turns a structure gs of type $\alpha G S$ into a graph system is the set of axioms it has to fulfill. All of these axioms are stated relative to $g s$. Because we have many axioms, it would be nice to state them as concise as possible. The Isabelle locale mechanism [1] fits our purpose. It allows entering a context in which chosen free


Figure 4.2: Planar Graph Record Components

| gs- $\sigma:: \alpha \Rightarrow$ real <br> gs- $\tau:$ <br> gs-ye $:: \alpha \Rightarrow$ real <br> gs-yn $:: \alpha \Rightarrow$ real <br> gs-sol $:: \alpha \Rightarrow$ real <br> gs-azim $:: \alpha \Rightarrow$ real | gs-tau-sigma $:: \alpha \Rightarrow$ real <br> gs-sigma-qrtet $:: \alpha \Rightarrow$ real <br> gs-sigma32-qrtet $:: \alpha \Rightarrow$ real <br> gs-sigma1-qrtet $:: \alpha \Rightarrow$ real | gs-sigma-quad $:: \alpha \Rightarrow$ real <br> gs-tau-quad $:: \alpha \Rightarrow$ real <br> gs-squad-quad $:: \alpha \Rightarrow$ real <br> gs-sol-quad $:: \alpha \Rightarrow$ real <br> gs-azim1-quad $:: \alpha \Rightarrow$ real <br> gs-azim2-quad $:: \alpha \Rightarrow$ real |
| :--- | :--- | :--- |

Figure 4.3: Real Variable Record Components
variables are fixed, that means within the context they are treated like constants, but are generalized on exiting the context. We choose gs as fixed variable and can then view all of the record components in Figures 4.2 and 4.3 as constants with a built-in implicit $g s$ parameter. In the locale context we define e.g.

$$
\sigma=g s-\sigma g s
$$

We introduce such an abbreviation for all of our record components and use these abbreviations from now on (except at those rare occasions where we look at a graph system from the outside).

### 4.2.1 Topology of a Graph System

Let us first make sense of the components shown in Figure 4.2. The leftmost box displays the components which model a planar graph in hypermap representation: the set of darts, and the edge, node and face permutations. We have no axioms actually enforcing that these ought to be permutations.

All other components displayed in Figure 4.2 are defined in terms of these 4 primitive components. The Face, Edge and Node functions assign to each dart its equivalence class. The definition of those functions listed in Figure 4.4 uses the notion of Orbit:

$$
\begin{equation*}
\text { Orbit } f s=\left\{f^{n} s \mid n \in \mathbb{N}\right\}=\{s, f s, f(f s), \ldots\} \tag{4.6}
\end{equation*}
$$

Sometimes we need to represent such an equivalence class by a single dart unique

$$
\begin{aligned}
& \text { Face }=\text { Orbit face } \\
& \text { Edge }=\text { Orbit edge } \\
& \text { Node }=\text { Orbit node }
\end{aligned}
$$

Figure 4.4: Axioms for Face, Edge and Node

$$
\begin{aligned}
\forall \alpha . \text { edgerep } \alpha & =\operatorname{Min}(\text { Edge } \alpha) \\
\forall \alpha . \text { facerep } \alpha & =\operatorname{Min}(\text { Face } \alpha) \\
\forall \alpha . \text { noderep } \alpha & =\operatorname{Min}(\text { Node } \alpha)
\end{aligned}
$$

Figure 4.5: Axioms for edgerep, facerep and noderep
to the class. This is why we require the type $\alpha$ of darts to be totally ordered: so that we can pick a single dart in a unique way out of each equivalence class. The edgerep, noderep and facerep functions assign to each dart the unique representing dart that belongs to the same equivalence class (fig. 4.5). We also want to be able to address all faces, or all edges, or all nodes. Thus, for each permutation, we form the set of all representatives of that permutation (fig. 4.6).

Finally, the rightmost box of Figure 4.2 is made up of further notions which enrich the topology related vocabulary of graph systems. Their definitions are listed in Figure 4.7.

### 4.2.2 3-Space Interpretation of a Graph System

To understand the real variable components of a graph system, it is helpful to recall how tame graphs originate from a packing of three-dimensional balls of radius 1 in 3-space. Given such a packing, pick any ball; this ball serves as the origin. Now select all balls the centers of which have a distance from the center of the origin of less than or equal to 2.51 . Connect then all such centers with straight lines if their distance is less than $2 t_{0}=2.51$. Project all of these lines onto the ball at the origin, and you have a spherical plane graph. After some normalization of this spherical plane graph you get a tame graph.

This means that a node of a tame graph corresponds to the center of a ball. And the edges of a tame graph correspond to the straight line connections between those centers. And the faces of a tame graph are basically a partitioning of the volume around the origin.

The real variable components refer to this 3-space interpretation of tame graphs. The real variable yn $\alpha$ interprets the dart $\alpha$ as a node; hence it must be invariant

$$
\begin{aligned}
\forall \alpha . \text { edges } & =\{\alpha \in \text { darts. edgerep } \alpha=\alpha\} \\
\forall \alpha . \text { faces } & =\{\alpha \in \text { darts. facerep } \alpha=\alpha\} \\
\forall \alpha . \text { nodes } & =\{\alpha \in \text { darts. noderep } \alpha=\alpha\}
\end{aligned}
$$

Figure 4.6: Axioms for edges, faces and nodes

```
            \forall \alpha \beta \text { . adjacent } \alpha \beta = ( \exists n \in \text { Node } \alpha \text { . edge } \alpha \in \text { Node } \beta )
\forall\beta. commonquad \alpha\beta=(\existsF\in Node \alpha. card (Face F)=4 and facerep F \in facerep 'Node \beta)
            \forall}\mathrm{ . separable }\alpha=(\operatorname{card}(\mathrm{ Node }\alpha)=5\mathrm{ and ( }\existsF\in\mathrm{ Node }\alpha.5\leq\operatorname{card (Face F)))
    \forall S \alpha . ~ s e p a r a b l e ' S ~ \alpha ~ = ~ ( s e p a r a b l e ~ \alpha ~ a n d ~ ( ~ \forall \beta \in S . \neg ~ ( a d j a c e n t ~ \alpha \beta ~ o r ~ c o m m o n q u a d ~ \alpha \beta ) ) )
                    \forall. tri \alpha = card (Node \alpha\cap{\beta.card (Face \beta})=3}
        \foralln. node-type \alpha n = (card (Node \alpha)=n\wedge(\forall\beta\inNode \alpha. card (Face }\beta)=3)
```

Figure 4.7: Further Topology Axioms
under the node permutation. It denotes the distance that the corresponding center of a ball has to the origin. Hence we have $2 \leq y n \alpha \leq 2 t_{0}$.

The real variable ye $\alpha$ interprets $\alpha$ as an edge. It is invariant under the edge permutation and measures the length of the straight line between two balls it corresponds to. Again, we have $2 \leq$ ye $\alpha \leq 2 t_{0}$.

The real variable sol $\alpha$ interprets $\alpha$ as a face. It measures the size of the area of the surface of the ball at the origin that this face corresponds to. It is invariant under the face permutation. Because the whole surface of a unit ball is $4 \pi$, we have $0 \leq \operatorname{sol} \alpha \leq 4 \pi$.

To explain the real variable azim $\alpha$, let us first interpret $\alpha$ as an arc on the surface of the ball at the origin. Applying the node permutation to $\alpha$ yields another dart $\alpha^{\prime}$ which we also interpret as such an arc. The two arcs have a point $p$ in common, the projection of the center of the ball that $\alpha$ corresponds to. Now azim $\alpha$ measures the spherical angle between those two arcs at $p$. Because azim $\alpha$ is an angle, we have $0 \leq \operatorname{azim} \alpha \leq 2 \pi$. We furthermore know the sum of all angles around a point:

$$
\begin{equation*}
\forall N \in \text { nodes. } 2 * \pi=\sum \alpha \in \text { Node } N . \operatorname{azim} \alpha \tag{4.7}
\end{equation*}
$$

In the plane, the sum of all inner angles of a triangle is $\pi$. For a spherical triangle, this is not true. Girard's Formula says that the difference between the sum of all inner spherical angles of a spherical triangle and $\pi$ is just the area of that spherical triangle. Generalizing this result to faces with $\geq 3$ edges gives:

$$
\begin{equation*}
\forall x \in \text { darts. sol } x=- \text { real }(\operatorname{card}(\text { Face } x)-2) * \pi+\sum \alpha \in \text { Face } x . \operatorname{azim} \alpha \tag{4.8}
\end{equation*}
$$

between the ends of that straight line and the origin.
The real variables $\sigma \alpha$ (the score) and $\tau \alpha$ are related to the density of the volume the face $\alpha$ corresponds to. They are connected via

$$
\begin{equation*}
\forall x \in \text { darts. } \tau x=\operatorname{sol} x * \zeta * p t-\sigma x \tag{4.9}
\end{equation*}
$$

where $p t=4 \arctan (\sqrt{2} / 5)-\frac{\pi}{3}$ and $\zeta=1 /(2 \arctan (\sqrt{2} / 5))$. For the graph system to be contravening, that is to qualify as part of a packing with highest possible density,

$$
\begin{equation*}
8 * p t \leq \sum \alpha \in \text { faces. } \sigma \alpha \tag{4.10}
\end{equation*}
$$

must hold.
The other real variables in the middle and rightmost box in Figure 4.3 are variations on the real variables in the first box; they are specified only in certain situations. Their relationship with the real variables from the first box is given by the axioms in Figure 4.11. The significance of these other variables lies in the existence of axioms which have been converted from a database of inequalities. See Appendix A for the complete list of these axioms.
$\forall x \in$ darts. $\sigma x=\sigma($ face $x)$
$\forall x \in$ darts. ye $x=$ ye $($ edge $x)$
$\forall x \in$ darts. yn $x=$ yn $($ node $x)$
$\forall x \in$ darts. sol $x=$ sol (face $x)$

Figure 4.8: Axioms for Invariance under Permutation

| $\forall x \in$ darts. $2 \leq$ yn $x$ | $\forall x \in$ darts. yn $x \leq 2 * t_{0}$ |
| :--- | :--- |
| $\forall x \in$ darts. $2 \leq$ ye $x$ | $\forall x \in$ darts. ye $x \leq 2 * t_{0}$ |
| $\forall x \in$ darts. $0 \leq$ azim $x$ | $\forall x \in$ darts. azim $x \leq 2 * \pi$ |
| $\forall x \in$ darts. $0 \leq \operatorname{sol} x$ | $\forall x \in$ darts. sol $x \leq 4 * \pi$ |

Figure 4.9: Axioms for Basic Geometrical Bounds

$$
\begin{aligned}
& \forall x \in \text { darts. card (Face } x \text { ) }=3 \text { implies } 0 \leq \tau x \\
& \forall x \in \text { darts. card (Face } x \text { ) }=4 \text { implies } 1317 / 10000 \leq \tau x \\
& \forall x \in \text { darts. card (Face } x \text { ) }=5 \text { implies } 27113 / 100000 \leq \tau x \\
& \forall x \in \text { darts. card (Face } x \text { ) }=6 \text { implies } 41056 / 100000 \leq \tau x \\
& \forall x \in \text { darts. card (Face } x \text { ) }=7 \text { implies } 54999 / 100000 \leq \tau x \\
& \forall x \in \text { darts. card (Face } x \text { ) }=8 \text { implies } 6045 / 10000 \leq \tau x \\
& \forall x \in \text { darts. card (Face } x \text { ) }=3 \text { implies } \sigma x \leq p t \\
& \forall x \in \text { darts. card (Face } x \text { ) }=4 \text { implies } \sigma x \leq 0 \\
& \forall x \in \text { darts. card (Face } x \text { ) }=5 \text { implies } \sigma x \leq-5704 / 100000 \\
& \forall x \in \text { darts. card (Face } x \text { ) }=6 \text { implies } \sigma x \leq-11408 / 100000 \\
& \forall x \in \text { darts. card (Face } x \text { ) }=7 \text { implies } \sigma x \leq-17112 / 100000 \\
& \forall x \in \text { darts. card (Face } x \text { ) }=8 \text { implies } \sigma x \leq-22816 / 100000
\end{aligned}
$$

Figure 4.10: Bounds for $\sigma$ and $\tau$ from [16, Lemma 20.2]

```
\(\forall x \in\) darts. card (Face \(x\) ) \(=3\) implies
    sigma32-qrtet \(x=\) sigma-qrtet \(x-32 / 10 * \zeta * p t * \operatorname{sol} x\)
\(\forall x \in\) darts. card (Face \(x\) ) \(=3\) implies
    sigma1-qrtet \(x=\) sigma-qrtet \(x-\zeta * p t * \operatorname{sol} x\)
\(\forall x \in\) darts. card (Face \(x\) ) \(=3\) implies \(\sigma x=\operatorname{sigma-qrtet} x \wedge \tau x=\) tau-sigma \(x\)
\(\forall x \in\) darts. card (Face \(x\) ) \(=4\) implies \(\sigma x=\operatorname{sigma-quad~} x\)
\(\forall x \in\) darts. card (Face \(x\) ) \(=4\) implies \(\tau x=\operatorname{tau}\)-quad \(x\)
\(\forall x \in\) darts. card (Face \(x\) ) \(=4\) implies squad-quad \(x=\sigma x \wedge\) sol-quad \(x=\operatorname{sol} x \wedge\)
    azim1-quad \(x=\operatorname{azim} x \wedge \operatorname{azim2-quad} x=\operatorname{azim}(\) face \(x)\)
```

Figure 4.11: Variations of Real Variables

```
\forall\alpha\in nodes. node-type \alpha 5 implies
    ( }\forall\beta\in\mathrm{ nodes. }\alpha<\beta\wedge\mathrm{ node-type }\beta5\mathrm{ implies
    (}\forall\gamma\in\mathrm{ nodes. }\beta<\gamma\wedge\mathrm{ node-type }\gamma5\mathrm{ implies
    (}\forall\delta\in\mathrm{ nodes. }\gamma<\delta\wedge\mathrm{ node-type }\delta5\mathrm{ implies
    55 / 100*4*pt\leq(\sumS faces \cap facerep'(Node \alpha\cupNode }\beta\cup\mathrm{ Node }\gamma\cupNode \delta).\tau S
    \wedge(\sumS faces \cap facerep'(Node }\alpha\cupNode \beta\cupNode \gamma\cupNode \delta).\sigmaS - pt)\leq-48 / 100*4*pt))
\forall\alpha\in nodes. node-type \alpha 5 implies
    (}\forall\beta\in\mathrm{ nodes. }\alpha<\beta\wedge\mathrm{ node-type }\beta5\mathrm{ implies
    (}\forall\gamma\in\mathrm{ nodes. }\beta<\gamma\wedge\mathrm{ node-type }\gamma5\mathrm{ implies
    55 / 100*3 * pt \leq (\sumS f faces \cap facerep '(Node \alpha \cup Node \beta\cup Node \gamma). \tau S)
    \wedge(\sumS faces \cap facerep '(Node }\alpha\cupNode \beta\cupNode \gamma).\sigmaS - pt)\leq-48 / 100*3*pt)
\forall\alpha\in nodes. node-type \alpha 5 implies
    (}\forall\beta\in\mathrm{ nodes. }\alpha<\beta\wedge\mathrm{ node-type }\beta5\mathrm{ implies
    55 / 100*2* pt \leq (\sumS faces \cap facerep '(Node \alpha\cup Node \beta).\tau S)
    \wedge(\sumS faces \cap facerep '(Node \alpha \cup Node \beta). \sigmaS - pt)\leq-48/100*2*pt)
\forall\alpha\in nodes. node-type \alpha 5 implies
    55 / 100 * 1 * pt \leq (\sumS S faces \cap facerep' Node \alpha.\tau S)
    \wedge(\sumS faces \cap facerep 'Node }\alpha.\sigmaS-pt)\leq-48/100*1*p
```

Figure 4.12: Axioms from [16, Lemma 10.6]
$\forall v_{1} \in$ nodes. separable $v_{1}$ implies
const-a (tri $\left.v_{1}\right) \leq\left(\sum F \in\right.$ faces $\cap$ facerep 'Node $v_{1} . \tau F / p t-$ const-d (card (Face $\left.F\right)$ ))
$\forall v_{1} \in$ nodes. separable $v_{1}$ implies
( $\forall v_{2} \in$ nodes. $v_{1}<v_{2}$ and separable ${ }^{\prime}\left\{v_{1}\right\} v_{2}$ implies
const-a $\left(\right.$ tri $\left.v_{1}\right)+$ const-a $\left(\right.$ tri $\left.v_{2}\right)$
$\leq\left(\sum F \in\right.$ faces $\cap$ facerep ' $\left(\right.$ Node $v_{1} \cup$ Node $\left.v_{2}\right) . \tau F / p t-\operatorname{const-d}(\operatorname{card}($ Face $\left.\left.F))\right)\right)$
$\forall v_{1} \in$ nodes. separable $v_{1}$ implies
( $\forall v_{2} \in$ nodes. $v_{1}<v_{2}$ and separable ${ }^{\prime}\left\{v_{1}\right\} v_{2}$ implies
$\left(\forall v_{3} \in\right.$ nodes. $v_{2}<v_{3}$ and separable' $\left\{v_{1}, v_{2}\right\} v_{3}$ implies
const-a $\left(\right.$ tri $\left.v_{1}\right)+$ const-a $\left(\right.$ tri $\left.v_{2}\right)+$ const-a $\left(\right.$ tri $\left.v_{3}\right)$
$\leq\left(\sum F \in\right.$ faces $\cap$ facerep ' $\left(\right.$ Node $_{1} \cup$ Node $v_{2} \cup$ Node $\left.v_{3}\right) . \tau F / p t-\operatorname{const-d}(\operatorname{card}($ Face $\left.\left.\left.F))\right)\right)\right)$

Figure 4.13: Axioms from [16, Lemma 22.12]

### 4.2.3 Additional Constraints of a Graph System

We are about to complete the specification of the axioms of a graph system. This subsection enumerates all axioms that are still missing.

First, this axiom is derived from [13, Group 4, rule 1]:

$$
\begin{equation*}
\forall \alpha \in \text { nodes. node-type } \alpha 4 \text { implies ( } \forall \beta \in \text { Node } \alpha . \sigma \beta \leq 33 / 100 * p t \text { ) } \tag{4.11}
\end{equation*}
$$

Second, here is an axiom derived from [13, Group 4, rule 3]:
$\forall \alpha \in$ nodes. node-type $\alpha 5$ implies

$$
\begin{equation*}
\left(\sum \beta \in \text { Node } \alpha \cdot \sigma \beta+419351 / 1000000 * \operatorname{sol} \beta-2856354 / 10000000\right) \leq 0 \tag{4.12}
\end{equation*}
$$

Finally, Figures 4.12 and 4.13 complete the set of axioms.
Thus we have defined the predicate GraphSystem of type $\alpha G S \Rightarrow$ bool which is true for some $g s$ if $g s$ fulfills all the axioms mentioned in Section 4.2.

### 4.3 Generating and Running the Basic Linear Programs

Each graph system axiom involving real variables is a generator for a set of linear inequalities in these real variables. For each tame graph, we assume that it fulfills all graph system axioms. We then run the axioms and produce a system of linear inequalities. If we are successful in showing that this system is infeasible, we have shown that the given tame graph cannot be a graph system, and thus constitutes no counter example to the Kepler conjecture.

We first need a connection between graph system and tame graph:

```
definition func-eq \(:: \alpha\) GS \(\Rightarrow(\alpha \Rightarrow \beta) \Rightarrow(\alpha \Rightarrow \beta) \Rightarrow\) bool
where
    func-eq gs \(f g=(\forall d . d \in g s\)-darts \(g s \longrightarrow f d=g d)\)
definition PGS :: nat GS \(\Rightarrow\) (nat \(\times\) nat \(\times\) nat \()\) NatTreeMap \(\Rightarrow\) bool
where
    PGS gs \(S=(\) GraphSystem gs
        \(\wedge\) gs-darts gs = dom (eval S)
        \(\wedge\) func-eq gs (gs-face gs) (map-face \(S\) )
        \(\wedge\) func-eq gs (gs-edge gs) (map-edge \(S\) )
        \(\wedge\) func-eq gs (gs-node gs) (map-node \(S\) ))
```

For a given tame graph $S$, say $S=$ graph-47, we can then enter the context $P G S$ gs $S$. The HOL Computing Library (HCL) allows us to perform computations within this context. If the HCL did not have that capability, it would have been impossible to apply the HCL to our problem, because all of our computations need to be done in a world which has the underlying implicit assumption PGS gs S. Our goal is to prove False in this world, thereby showing that this is a world which is not real.

How do we execute an axiom? First note that by linking graph system and tame graph, the permutation functions of the graph system become executable. We provide theorems to the HCL such that from the executability of the permutation functions the executability of all axioms follows.

Say the axiom has the form

$$
\forall x \in B . P x
$$

If $B$ is a finite set such that $B=\left\{b_{1}, \ldots, b_{n}\right\}$, then executing this axiom means converting it into the form $P b_{1} \wedge \ldots \wedge P b_{n}$. In our situation, $B$ is often given as the orbit of a permutation function, for example $B=$ Orbit face $d$. Then executing the axiom results in

$$
P d \wedge P(\text { face } d) \wedge P(\text { face }(\text { face } d)) \wedge \ldots
$$

where the conjunction is finite if the orbit is. The nice thing about finite orbits is therefore that they come with a built-in traversal strategy, i.e. we know how to visit every element of the set exactly once. If $X$ is a set with such a traversal strategy, and $Y$ is a set such that the membership test $y \in Y$ is executable (which is e.g. true if $Y$ has a traversal strategy), then $X \cap Y$ has also a traversal strategy: just follow the traversal strategy of $X$, skipping elements if they are not in $Y$. Of course,then $X-Y$ also has a traversal strategy: follow the one of $X$, skipping elements if they are in $Y$. The case $X \cup Y$ is problematic, even if both $X$ and $Y$ have a traversal strategy. Our solution in this situation is to find a set $C$ with traversal strategy such that $X \cup Y=C \cap(X \cup Y)$. Then $C \cap(X \cup Y)$ is clearly traversable because $C$ has a traversal
strategy and the membership test for $X \cup Y$ is executable. All of the sets in our application are subsets of darts. If darts is a traversable set, then this reformulation is always possible. Note that although the requirement to visit an element not more than once is not really necessary for executing $\forall$, it is nevertheless essential for executing $\sum$.

We showed in [28] how to define and reason about functions on orbits with the help of the While and For combinators. Using the techniques presented there we have defined a fold functional for orbits, and proven theorems about the relationship of that fold functional with the one for finite sets presented in [24]. This allowed us to reuse many results already available in Isabelle, for example when making the Min function executable on orbits, which is needed for making facerep etc. executable.

In many axioms we used instead of the normal implication operator $\longrightarrow$ the short-circuit operator implies (fig. 2.10). Note that this is essential in order to be able to execute certain axioms like those in Figure 4.12 or 4.13 in reasonable time.

The result of executing a graph specification is a large conjunction of equalities and inequalities. We perform a normalization step to turn this large conjunction into matrix form. We then approximate the matrix by the method mentioned in Section 3.7.4. After this, we calculate a priori bounds as explained in Section 3.8. Then the linear program is ripe for trying to prove its infeasibility. Applying the method of Section 3.5, we manage to prove False for about $92.5 \%$ of all tame graphs. For example, for the tame graph graph-47 we prove

$$
\text { PGS gs graph- } 47 \Longrightarrow \text { False }
$$

Detailed results are listed in Appendix B. Let's do a quick sanity check. The number of the tame graph corresponding to the face-centered cubic packing is 901, the number of the one corresponding to the hexagonal-close packing is 880. Looking both numbers up shows that our methods failed for them, we could not prove PGS gs graph $-880 \Longrightarrow$ False or $P G S$ gs graph $-901 \Longrightarrow$ False. And that is how it should be.

Future work is to look at more complicated linear programs than the basic linear programs, and thereby to extend the methods presented in this thesis to tackle the remaining tame graphs.

## Graph System Axioms from the Inequality Database

This appendix lists those graph system axioms which have been converted from the database of inequalities which can be retrieved as HOL-light specification from [11].

The axioms are either for triangular faces, or for quadrilateral faces. For triangular faces, they hold for a face $F$ under the assumption tetra-bound $F$, for quadrilateral faces they hold under the assumption quad-bound $F$. These predicates are local to the graph system specification and not exported, their definition is:

```
tetra-bound F \equiv
    card (Face F)=3
\wedge 2\leqyn F^ yn F \leq 251/100
\wedge < yn (face F)^ yn (face F)\leq251/100
\wedge 2\leqyn (face (face F)) ^ yn (face (face F)) \leq251/100
\wedge < ye (face F) ^ ye (face F)\leq251/100
\wedge 2\leq ye (face (face F)) ^ ye (face (face F)) \leq251/100
\wedge 2\leqye F^ ye F\leq251/100
quad-bound F\equiv
    card (Face F) = 4
\wedge 2\leqyn F^ yn F\leq251/100
\wedge 2\leqyn (face F) ^ yn (face F)\leq251/100
\wedge 2\leqyn (face (face F)) ^ yn (face (face F)) \leq251/100
\wedge 2\leqyn (face (face (face F))) ^ yn (face (face (face F))) \leq251/100
\wedge < ye (face F) ^ ye (face F) \leq251/100
\wedge 2\leq ye (face (face F)) ^ ye (face (face F))\leq251/100
\wedge 2\leq ye (face (face (face F))) ^ ye (face (face (face F))) \leq251/100
\wedge 2 \leq ye F ^ ye F\leq251/100
```

Because in this thesis we look only at graph systems corresponding to basic linear programs, the definitions could actually be expressed in a simpler way:
tetra-bound $F \equiv \operatorname{card}($ Face $F)=3$
quad-bound $F \equiv \operatorname{card}($ Face $F)=4$

| $\mathrm{J}_{16189133}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-1369 / 10000+$ sigma32-qrtet $x+1966 / 10000$ |
| :---: | :---: |
| $\mathrm{J}_{49987949}$ | $\begin{aligned} & \forall x \in \text { darts. tetra-bound } x \longrightarrow \\ & 190249 / 1000000+\text { sigma-qretet } x+-446634 / 1000000 * \text { sol } x<0 \end{aligned}$ |
| $\mathrm{J}_{53415898}$ | $\forall x \in$ darts. tetra-bound $x \rightarrow$ sigma1-qrtet $x \leq 0$ |
| $\mathrm{J}_{73203677}$ | $\begin{aligned} & \forall x \in \text { darts. tetra-bound } x \longrightarrow-13225 / 10000+\text { sigma-qrtet } x+419351 / 1000000 * \text { sol } x+ \\ & 64713719 / 100000000 * \operatorname{azim} x<0 \end{aligned}$ |
| $\mathrm{J}_{98170671}$ | $\begin{aligned} & \forall x \in \text { darts. tetra-bound } x \longrightarrow-2114190 / 10000000+\operatorname{sigma-qrtet} x+419351 / 1000000 * \operatorname{sol} x \\ & +-610397 / 10000000 * \operatorname{azim} x<0 \end{aligned}$ |
| $\mathrm{J}_{106537269}$ | $\forall x \in$ darts. tetra-bound $x \rightarrow-208 / 1000+$ sigma1-qrtet $x+1689 / 10000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{170403135}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 5974 / 10000+$ sigma32-qrtet $x+-4233 / 10000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{195296574}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 45 / 10000+$ sigma32-qrtet $x+953 / 10000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{208809199}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 8638 / 10000-\operatorname{azim} x<0$ |
| $\mathrm{J}_{221945658}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 3683 / 10000+$ sigma1-qrtet $x+-2993 / 10000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{254627291}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-3442 / 10000+$ sigma1-qrtet $x+2529 / 10000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{382430711}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 4582620 / 10000000+$ sol $x+-320937 / 1000000 *$ ye (face $x)+$ $-320937 / 1000000 *$ ye $($ face $($ face $x))+-320937 / 1000000 *$ ye $x+152679 / 1000000 *$ yn $x+$ $152679 / 1000000 *$ yn $($ face $x)+152679 / 1000000 *$ yn $($ face $($ face $x))<0$ |
| $\mathrm{J}_{507227930}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 651760 / 10000000+\operatorname{azim} x+153598 / 1000000 *$ yn (face $x)+$ $153598 / 1000000 *$ yn $($ face $($ face $x))+153598 / 1000000 *$ ye $($ face $($ face $x))+153598 / 1000000$ * ye $x+-498 / 1000 *$ yn $x+-76446 / 100000 *$ ye $($ face $x)<0$ |
| $\mathrm{J}_{539256862}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 41110 / 100000+$ sigma-qrtet $x+-37898 / 100000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{544014470}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 16183310 / 10000000+199235 / 1000000 *$ ye (face $x)+199235$ <br> $/ 1000000 *$ ye $($ face $($ face $x))+199235 / 1000000 *$ ye $x+-377076 / 1000000 *$ yn $x+-377076$ <br> / $1000000 *$ yn $($ face $x)+-377076 / 1000000 *$ yn $($ face $($ face $x))-\operatorname{sol} x<0$ |
| $\mathrm{J}_{568731327}$ | $\begin{aligned} & \forall x \in \text { darts. tetra-bound } x \longrightarrow 27341020 / 10000000+-359894 / 1000000 * \text { yn }(\text { face } x)+ \\ & -359894 / 1000000 * \text { yn }(\text { face }(\text { face } x))+-359894 / 1000000 * \text { ye }(\text { face }(\text { face } x))+-359894 / \\ & 1000000 * \text { ye } x+3 / 1000 * \text { yn } x+685 / 1000 * \text { ye }(\text { face } x)-\operatorname{azim} x<0 \end{aligned}$ |
| $\mathrm{J}_{584511898}$ | $\begin{aligned} & \forall x \in \text { darts. tetra-bound } x \rightarrow 5786316 / 10000000+\text { sigma-qrtet } x+419351 / 1000000 * \text { sol } x \\ & +-796456 / 1000000 * \operatorname{azim} x<0 \end{aligned}$ |
| $\mathrm{J}_{586468779}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-p t+$ sigma-qrtet $x \leq 0$ |
| $\mathrm{J}_{649712615}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-128213260 / 100000000+$ sigma1-qrtet $x+129119 / 1000000$ * ye $($ face $x)+129119 / 1000000 *$ ye $($ face $($ face $x))+129119 / 1000000 *$ ye $x+845696 /$ $10000000 * y n x+845696 / 10000000 * y n($ face $x)+845696 / 10000000 * y n($ face $($ face $x))<0$ |
| $\mathrm{J}_{710947756}$ | $\begin{aligned} & \forall x \in \text { darts. tetra-bound } x \longrightarrow-1486650 / 1000000+\text { sigma-qrtet } x+419351 / 1000000 * \text { sol } x \\ & +2 / 10 * y n x+2 / 10 * \text { yn }(\text { face } x)+2 / 10 * y n(\text { face }(\text { face } x))<0 \end{aligned}$ |
| $\mathrm{J}_{776305271}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-5353 / 10000+$ sigma-qrtet $x+3302 / 10000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{789045970}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-13582137 / 10000000+$ sigma-qrtet $x+10857 / 100000 *$ yn $x$ $+10857 / 100000 *$ yn $($ face $x)+10857 / 100000 *$ yn $($ face $($ face $x))+10857 / 100000 *$ ye (face $x)+10857 / 100000 *$ ye $($ face $($ face $x))+10857 / 100000 *$ ye $x<0$ |
| $\mathrm{J}_{802409438}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 2550 / 10000+$ sigma32-qrtet $x+-1083 / 10000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{809197575}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-35641 / 100000+$ sigma-qrtet $x+419351 / 1000000 *$ sol $x+$ 499559 / $10000000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{825495074}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-2866354 / 10000000+$ sigma-qrtet $x+419351 / 1000000 * \operatorname{sol} x<0$ |
| $\mathrm{J}_{864218323}$ | $\forall x \in$ darts. tetra-bound $x \rightarrow-23021 / 100000+$ sigma-qrtet $x+142 / 1000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{868828815}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-308526 / 1000000+$ sigma-qrtet $x+419351 / 1000000 * \operatorname{sol} x+$ $162028 / 10000000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{927432550}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow 4666 / 10000+$ sigma1-qrtet $x+-3897 / 10000 * \operatorname{azim} x<0$ |
| $\mathrm{J}_{984463800}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow-1874445 / 1000000+\operatorname{azim} x<0$ |
| $\mathrm{J}_{995444025}$ | $\forall x \in$ darts. tetra-bound $x \longrightarrow$ <br> $-287389 / 1000000+\operatorname{sigma-qrtet} x+37642101 / 100000000 * \operatorname{sol} x<0$ |


| $\mathrm{J}_{15141595}$ | $\forall x \in$ darts. quad-bound $x \rightarrow 6284 / 10000+$ squad-quad $x+-3878 / 10000 *$ azim1-quad $x<0$ |
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| $\mathrm{J}_{18502666}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 166174 / 100000+$ squad-quad $x+419351 / 1000000 *$ sol-quad $x+-1582508 / 1000000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{73283761}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 8341 / 10000+$ squad-quad $x+-5301 / 10000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{122375455}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow$ $2955 / 1000+$ squad-quad $x+-(p t * \zeta) *$ sol-quad $x+-21406 / 10000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{153920401}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 4893 / 1000+$ squad-quad $x+-(32 / 10 * p t * \zeta) *$ sol-quad $x$ + -35294 / 10000 * azim1-quad $x<0$ |
| $\mathrm{J}_{166451608}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow-41717 / 100000+$ squad-quad $x+3 / 10 *$ sol-quad $x<0$ |
| $\mathrm{J}_{277330628}$ | $\forall x \in$ darts. quad-bound $x \rightarrow-3247 / 1000+$ azim1-quad $x<0$ |
| $\mathrm{J}_{310151857}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow$ <br> $57906 / 10000+$ squad-quad $x+-456766 / 100000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{322621318}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 9494 / 1000+$ squad-quad $x+-30508 / 10000 *$ azim1-quad $x$ $+-30508 / 10000 *$ azim2-quad $x<0$ |
| $\mathrm{J}_{337637212}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 4126 / 10000+$ squad-quad $x+-(32 / 10 * p t * \zeta) *$ sol-quad $x<0$ |
| $\mathrm{J}_{393682353}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow-3825 / 10000+$ squad-quad $x+-(p t * \zeta) *$ sol-quad $x+2365$ / 10000 * azim1-quad $x<0$ |
| $\mathrm{J}_{396281725}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow-15707 / 10000+$ squad-quad $x+5905 / 10000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{408478278}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 6438 / 10000+$ squad-quad $x+-(p t * \zeta) *$ sol-quad $x+-316 /$ $1000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{444643063}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 10472 / 10000+$ squad-quad $x+-27605 / 100000 *$ azim1-quad $x+-27605 / 100000 *$ azim2-quad $x<0$ |
| $\mathrm{J}_{465497818}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 5350181 / 1000000+$ squad-quad $x+419351 / 1000000 *$ sol-quad $x+-4611391 / 1000000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{539320075}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 581446 / 100000+$ squad-quad $x+-(p t * \zeta) *$ sol-quad $x+$ -449461 / $100000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{552698390}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow-35926 / 10000+$ squad-quad $x+844 / 1000 *$ azim1-quad $x+$ 844 / $1000 *$ azim2-quad $x<0$ |
| $\mathrm{J}_{574391221}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow-4124 / 10000+$ squad-quad $x+1897 / 10000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{616145964}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 577942 / 100000+$ squad-quad $x+-(32 / 10 * p t * \zeta) *$ sol-quad $x+-425863 / 100000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{655029773}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow$ <br> $20749 / 10000+$ squad-quad $x+-15094 / 10000 * \operatorname{azim1-quad} x<0$ |
| $\mathrm{J}_{657406669}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 1153 / 1000-\operatorname{azim1-quad} x<0$ |
| $\mathrm{J}_{676439533}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow-895 / 10000+$ squad-quad $x+419351 / 1000000 *$ sol-quad $x$ $+-342747 / 1000000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{768057794}$ | $\begin{aligned} & \forall x \in \text { darts. quad-bound } x \longrightarrow-33 / 100+\text { squad-quad } x+-(32 / 10 * p t * \zeta) * \text { sol-quad } x+ \\ & 316 / 1000 * \text { azim1-quad } x<0 \end{aligned}$ |
| $\mathrm{J}_{775642319}$ | ```\forallx\in darts.quad-bound x}\longrightarrow-1071/1000 + squad-quad x+-(pt*\zeta)*sol-quad x + 4747 / 10000 * azim1-quad x <0``` |
| $\mathrm{J}_{974296985}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow-336909 / 100000+$ squad-quad $x+419351 / 1000000 *$ sol-quad $x+974137 / 1000000 *$ azim1-quad $x<0$ |
| $\mathrm{J}_{996268658}$ | $\forall x \in$ darts. quad-bound $x \longrightarrow 1317 / 10000+$ squad-quad $x+-(p t * \zeta) *$ sol-quad $x<0$ |

## APPENDIX $\mathbf{B}$

## Results of Running the Basic LPs

In this appendix we list our results of running our methods on the archive of tame graphs. For each tame graph, we assumed that it forms a graph system. By generating the corresponding basic linear program and trying to prove it infeasible we tried to show that this assumption was false. Our results are presented in tables of the following format:

| \# | Inconsistent | Time |
| :--- | :--- | :--- |
|  |  |  |

The ' $\#$ ' column contains the number of the tame graph that has been examined. The numbering is chosen to correspond to the order of the tame graphs listed in [22]. A tame graph is in class $n$ if all of its faces have at most $n$ edges and there is at least one face with $n$ edges. Class 3 ranges from \#1 to \#20, class 4 from \#21 to \#943, class 5 from \#944 to \#2488, class 6 from \#2489 to \#2726, class 7 from \#2727 to \#2749, and class 8 from \#2750 to \#2771.

The 'Inconsistent' column says 'Yes' if we have successfully shown the infeasibility of the basic linear program induced by the tame graph, and therefore shown the inconsistency of the corresponding graph system. If it says '?', we only know that our methods failed on this graph.

Finally, the 'Time' column tells us how many minutes the examination of the tame graph lasted. We used the SML mode of the HOL Computing Library. Each tame graph has been examined by its own Isabelle process. Each Isabelle process ran on a dedicated processor of a cluster of 32 four processor 2.4 GHz Opteron 850 machines with 8 GB RAM per machine. The quickest process needed 8.4 minutes, the slowest 67 . The examination of all tame graphs took about 7.5 hours of cluster runtime. This corresponds to about 40 days on a single processor machine.

We were able to prove the inconsistency of 2565 of the graph systems, and failed on 206. This yields a success rate of about $92.5 \%$.





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[^1]:    ${ }^{1}$ The true content of this statement probably is: there is a way to implement the HCL correctly.

[^2]:    ${ }^{2}$ test could also have been defined via fun test $\mathrm{x}=$ (norm $\mathrm{x}=$ Zero)

[^3]:    ${ }^{3}$ In our setting there is always such a $t^{\prime}$ because $t$ can be simply typed. Otherwise, just say that the SML machine fails on any input.

[^4]:    ${ }^{4}$ This is not exactly how it works in Isabelle, but good enough for our purposes.

[^5]:    ${ }^{5}$ we assume atoms $(t) \subseteq \operatorname{dom} \sigma$, otherwise $\sigma$ is for the duration of the computation extended to an encoding $\sigma^{\prime}$ which has this property

[^6]:    ${ }^{1}$ Here and in the following we deviate slightly from actual Isabelle/HOL syntax for various reasons, the most important being formatting; the actual Isabelle/HOL user will have no difficulty translating the given theory snippets to proper Isabelle/HOL syntax.

[^7]:    ${ }^{2}$ Our convention is that left distributivity means that the factor is distributed over the left sum, not that the left factor is the one that gets distributed.

