

Verified Computer Linear Algebra¹

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DE LA RIOJA**

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Introduction

Gauss-Jordan

QR Decomposition

Conclusions

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 - ▶ the available tools in Isabelle/HOL

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- ▶ The optimised version is generated to functional languages, and applied to case studies

Toolkit

- ▶ Proof assistant: Isabelle (L. Paulson, T. Nipkow, M. Wenzel)
- ▶ Underlying logic: Higher-order logic (HOL) + type classes
- ▶ Additional libraries: HOL Multivariate Analysis (HMA, J. Harrison)
- ▶ Code generation infrastructure (F. Haftmann)
- ▶ Proof language: Intelligible semi-automated reasoning (Isar, M. Wenzel)
- ▶ Execution environments: GH(askell)C, PolyML (D. Matthews) and MLton

HMA - Multivariate Analysis session

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typedef (α, β) vec = UNIV :: $((\beta::\text{finite}) \Rightarrow \alpha)$ set
morphisms vec-nth vec-lambda ..

- ▶ Type System vs Logic

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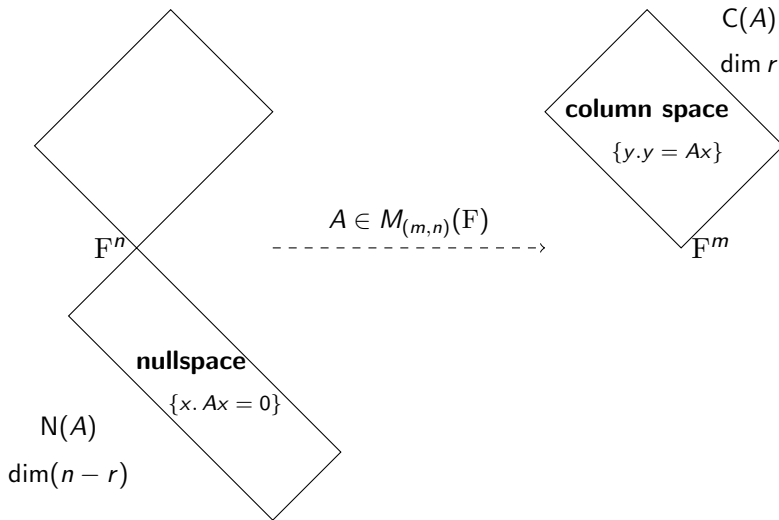


Figure : Rank Nullity Theorem

From theorems to algorithms

- ▶ Gauss-Jordan elimination provides a direct way to compute $\dim(C(A))$ by means of *elementary row operations* over $A \in M_{(m,n)}(F)$

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Gauss-Jordan example

$$A = \begin{pmatrix} 1 & -2 & 1 & -3 & 0 \\ 3 & -6 & 2 & -7 & 0 \\ 5 & -1 & 3 & 2 & 5 \\ 0 & 7 & 4 & 5 & 1 \\ 3 & -6 & 2 & -7 & 0 \end{pmatrix} \longrightarrow A = \begin{pmatrix} 1 & 0 & 0 & 0 & 3 \\ 0 & 1 & 0 & 0 & 2 \\ 0 & 0 & 1 & 0 & -2 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

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$$\dim(\mathcal{C}(A)) = 4$$

Elementary operations

Most Linear Algebra algorithms can be implemented using exclusively elementary row (column) operations on matrices, *i.e.*

Elementary row (column) operations

- ▶ Interchange two different rows (columns)
- ▶ Multiply a row (column) by an invertible element
- ▶ Add to a row (column) another one multiplied by a constant

We have implemented these operations and their properties in Isabelle. These are later on used to formalise, execute and refine algorithms.

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Gauss-Jordan algorithm applications

- ▶ Ranks
- ▶ Determinants
- ▶ Inverses
- ▶ Dimensions and bases of the null space, left null space, column space and row space
- ▶ Solution(s) of systems of linear equations

Relying on *invariants*

Elementary row operations do not modify, or modify in a predictable way, the previous computations

Isabelle lemmas about elementary operations

lemma crk-is-preserved:

fixes $A::\text{real}^{\text{'cols::}\{\text{finite, wellorder}\}^{\text{'rows}}}$ **and** $P::\text{real}^{\text{'rows}^{\text{'rows}}}$

assumes inv-P: invertible P

shows $\text{col-rank } A = \text{col-rank } (P ** A)$

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lemma det-mult-row:

shows $\det (\text{mult-row } A \text{ a } k) = k * \det A$

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lemma matrix-inv-Gauss-Jordan-PA:

fixes $A::\text{real}^{\text{'n}}::\{\text{mod-type}\}^{\text{'n}}::\{\text{mod-type}\}$

assumes inv-A: invertible A

shows $\text{matrix-inv } A = \text{fst } (\text{Gauss-Jordan-PA } A)$

Relying on the properties of Gauss-Jordan

Isabelle lemmas to compute the previous properties

definition basis-null-space A =

$\{\text{row } i \text{ (P-Gauss-Jordan (transpose A))} \mid i. \text{ to-nat } i \geq \text{rank } A\}$

definition basis-row-space A =

$\{\text{row } i \text{ (Gauss-Jordan A)} \mid i. \text{ row } i \text{ (Gauss-Jordan A)} \neq 0\}$

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definition solve-system A b =

$(\text{let } GJ = \text{Gauss-Jordan-PA } A \text{ in } (\text{snd } GJ, (\text{fst } GJ) * v \text{ b}))$

definition solve A b = (if consistent A b then

Some (solve-consistent-rref (fst (solve-system A b)) (snd (solve-system A b)),
basis-null-space A)
else None)

Refinement

Abstract representation

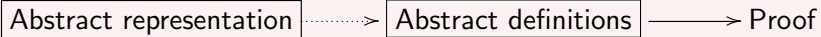
Refinement

Abstract representation $\rightarrow$

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Abstract representation $\dashv\dashv$ Abstract definitions

Refinement



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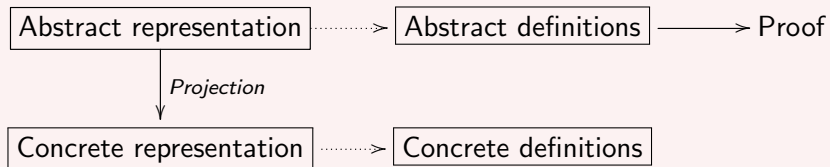
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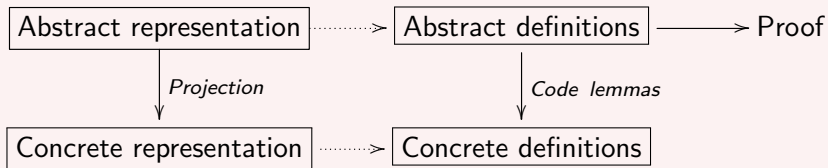
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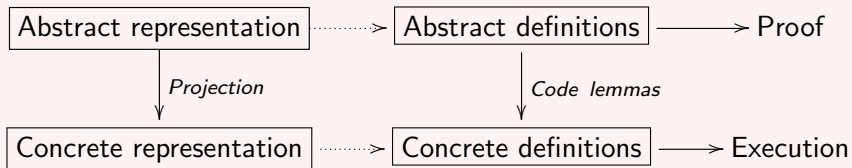
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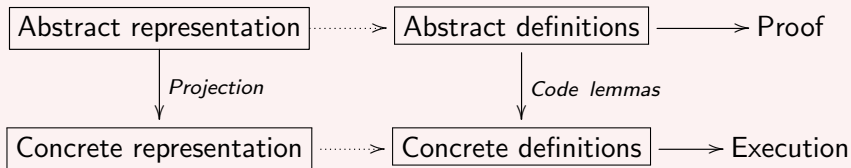
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Refinement



A refinement has been carried out so that operations over the abstract type *vec* can be executed

1. Mapping *vec* to *iarray*

From `vec` to `iarray`

In order to achieve better performance, a new refinement has been developed using immutable arrays

- ▶ There exists a datatype in the Isabelle library called *iarray* which represents immutable arrays
- ▶ *iarray* is implemented in both SML (*Vector structure*) and Haskell (*IArray class*)
- ▶ We have refined *vec* elements and operations to *iarray* ones (proving the corresponding morphisms)

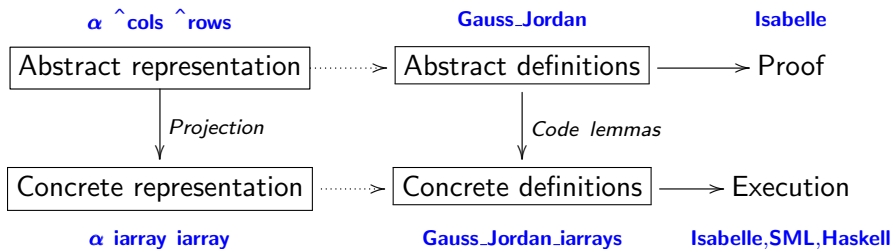
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Features of this refinement

1. Code can be generated to both SML and Haskell
2. Both *vec* and *iarray* have a similar functional flavour (for instance, in access operations)



Serialisations

Isabelle/HOL	SML	Haskell
<i>iarray</i>	<i>Vector.vector</i>	IArray.Array
<i>rat</i>	<i>IntInf.int / IntInf.int</i>	Rational
<i>real</i>	<i>Real.real</i>	Double
<i>bit</i>	Bool.bool	Bool

Table : Type serialisations

Judgement Day

Size (n)	Poly/ML	MLton	GHC
100	0.04	0.05	0.36
200	0.25	0.32	2.25
400	2.01	2.35	17.17
800	15.96	18.57	131.73
1 200	62.33	70.45	453.57
1 600	139.70	152.41	1097.41
2 000	284.28	287.44	2295.30

Table : Elapsed time (in seconds) to compute the *rref* of randomly generated $\mathbb{Z}_2^{n \times n}$ matrices using iarrays

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Some relevant facts

- ▶ Both in SML and GHC we have serialised $\mathbb{Z}_2$ to *bool*

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- ▶ Compilation in GHC is performed using compilation optimisations such as `-o3` (<https://wiki.haskell.org/Performance/GHC>)

Judgement Day

Size (n)	Poly/ML	Haskell
10	0.01	0.01
20	0.02	0.03
40	0.21	0.24
60	1.16	1.09
80	3.77	3.53
100	9.75	9.03

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- ▶ In SML we have serialised $\mathbb{Q}$ to quotients of *IntInf.int*
- ▶ In GHC we have serialised $\mathbb{Q}$ to *Rational*

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- ▶ Both Poly/ML and GHC internally use GMP (<https://gmplib.org/>) to enhance performance
- ▶ We have optimised SML code by using some particular serialisations (computing the Isabelle *divmod* is done in Poly/ML by means of *IntInf.quotrem*)

Judgment Day

Size (n)	Poly/ML	Haskell
100	0.03	0.38
200	0.25	2.62
300	0.81	8.47
400	1.85	19.51
500	3.51	37.13
600	6.03	64.13
700	9.57	100.59
800	13.99	148.20

Table : Time to compute the *rref* of randomly generated $\mathbb{R}$ matrices.

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Some relevant facts

- ▶ In SML we have serialised $\mathbb{R}$ to *Real.real*
- ▶ In GHC we have serialised $\mathbb{R}$ to *Prelude.Double* (see for instance http://www.isa-afp.org/browser_info/current/AFP/Gauss_Jordan/Code_Real_Approx_By_Float_Haskell.html)

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- ▶ WARNING: use the obtained code at your own risk



C++ vs Verified version

Matrix sizes	C++ version	Verified version
600×600	01.33s.	06.16s.
$1\,000 \times 1\,000$	05.94s.	32.08s.
$1\,200 \times 1\,200$	10.28s.	62.33s.
$1\,400 \times 1\,400$	16.62s.	97.16s.

Table : C++ vs verified version of the Gauss-Jordan algorithm.

Both programs show a cubic performance, even if the verified version is using immutable arrays

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Theorem (Second Part of the Fundamental Theorem of Linear Algebra)

Given a matrix $A \in M_{(m,n)}(\mathbb{R})$

- ▶ In $\mathbb{R}^n$, $N(A) = C(A^T)^\perp$ that is, the nullspace is the orthogonal complement of the row space

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- ▶ In $\mathbb{R}^m$, $N(A^T) = C(A)^\perp$, that is, the left nullspace is the orthogonal complement of the column space

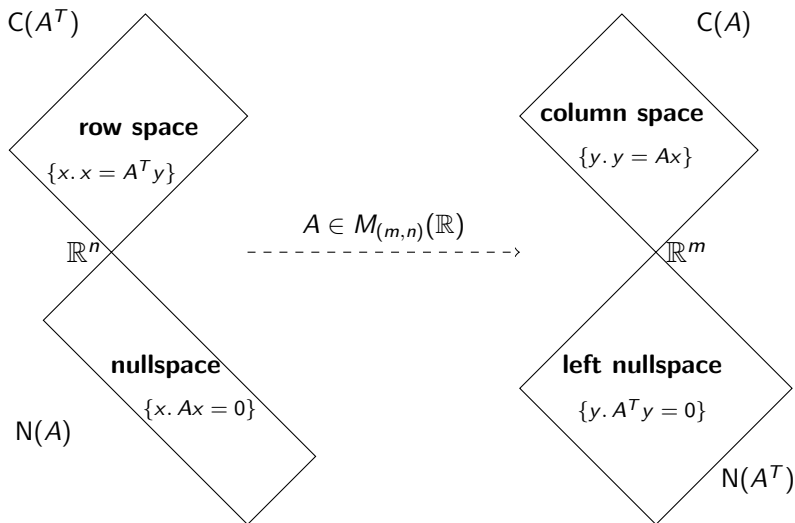


Figure : Orthogonality of the Four Fundamental subspaces

Second Part of the Fundamental Theorem of Linear Algebra

- ▶ **theorem** null-space-orthogonal-complement-row-space:
fixes $A :: \text{real}^{\text{'cols'}} \text{'rows'}$
shows null-space $A = \text{orthogonal-complement (row-space } A)$

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From Mathematical results to algorithms

The *Gram-Schmidt process* allows us to compute the mentioned orthogonal bases

QR decomposition

Definition (QR decomposition)

The QR decomposition of a full column rank matrix $A \in M_{n \times m}(\mathbb{R})$ is a pair of matrices (Q, R) such that

1. $A = QR$
2. $Q \in M_{n \times m}(\mathbb{R})$ is a matrix whose columns are orthonormal vectors
3. $R \in M_{m \times m}(\mathbb{R})$ is upper triangular and invertible

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Algorithm

1. $Q =$ Apply Gram-Schmidt to the columns of A , normalise the vectors
2. Compute R as $R = Q^T A$

QR Decomposition

- ▶ We have formalised the previous algorithm in Isabelle, and refined it to immutable arrays
- ▶ Computations can be carried out using either floats or (for suitable inputs) symbolically

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René Thiemann. Implementing field extensions of the form $\mathbb{Q}[\sqrt{b}]$.

Archive of Formal Proofs (2014)

QR Decomposition

definition $A :: \text{real}^4^4$

where `foo` = `list-of-list-to-matrix` $\begin{bmatrix} [1,2,4,6], \\ [9,4,5,2], \\ [0,0,4,3], \\ [3,2,4,1] \end{bmatrix}$

value `matrix-to-list-of-list` (`show-matrix-real` (`fst` (`QR-decomposition` A)))

output

$\begin{bmatrix} [1/91\sqrt{91}, 69/5642\sqrt{5642}, -9/15934\sqrt{15934}, 6/257\sqrt{257}], \\ [9/91\sqrt{91}, -8/2821\sqrt{5642}, -3/7967\sqrt{15934}, 4/257\sqrt{257}], \\ [0, 0, 2/257\sqrt{15934}, 3/257\sqrt{257}], \\ [3/91\sqrt{91}, 25/5642\sqrt{5642}, 21/15934\sqrt{15934}, -14/257\sqrt{257}] \end{bmatrix}$
`:: char list list list`

QR decomposition

value matrix-to-list-of-list (show-matrix-real (snd (QR-decomposition A)))

output

```
[[sqrt(91), 44/91*sqrt(91), 61/91*sqrt(91), 27/91*sqrt(91)],
 [ 0, 2/91*sqrt(5642), 148/2821*sqrt(5642), 407/5642*sqrt(5642)],
 [ 0, 0, 1/31*sqrt(15934), 327/15934*sqrt(15934)],
 [ 0, 0, 0, 39/257*sqrt(257)]] :: char list
list list
```

value A == (fst (QR-decomposition A)) ** (snd (QR-decomposition A))

output True :: prop

Application: Least Squares Approximation

- ▶ Let us consider a system $Ax = b$ without solution
- ▶ We can approximate the solution minimizing the error (least squares approximation). That is, compute $\hat{x}$ such that minimises $\| A\hat{x} - b \|$

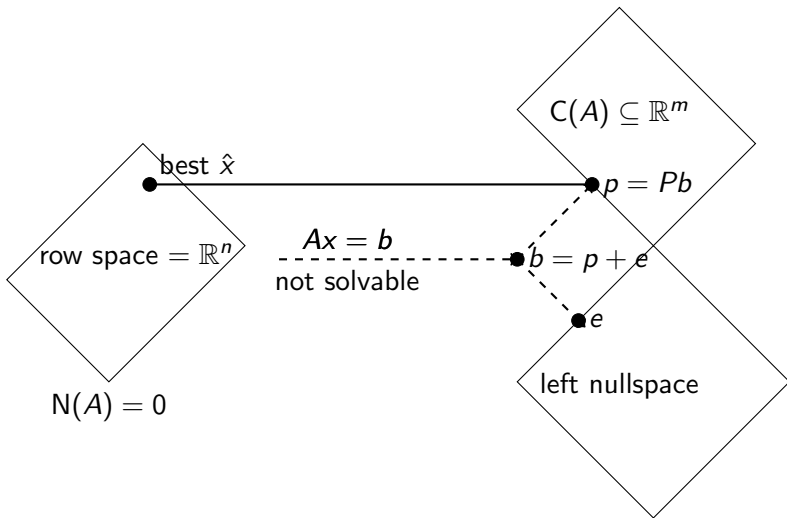


Figure : The projection $p = A\hat{x}$ is the closest point to b in $C(A)$

Application: Least Squares Approximation

- ▶ We have formalised that $\hat{x} = R^{-1}Q^T b$
- ▶ $\hat{x}$ can be computed symbolically, R^{-1} is computed by means of the Gauss-Jordan algorithm

Judgment day (using rationals for $\mathbb{R}$)

$$H_6 x = b$$

$$H_6 = \begin{pmatrix} 1 & 1/2 & 1/3 & 1/4 & 1/5 & 1/6 \\ 1/2 & 1/3 & 1/4 & 1/5 & 1/6 & 1/7 \\ 1/3 & 1/4 & 1/5 & 1/6 & 1/7 & 1/8 \\ 1/4 & 1/5 & 1/6 & 1/7 & 1/8 & 1/9 \\ 1/5 & 1/6 & 1/7 & 1/8 & 1/9 & 1/10 \\ 1/6 & 1/7 & 1/8 & 1/9 & 1/10 & 1/11 \end{pmatrix}, b = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 5 \end{pmatrix}$$

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The least squares approximation

$$x = [-13824, 415170, -2907240, 7754040, -8724240, 3489948]$$

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Performance

- ▶ Poly/ML with optimisations: 0.013 s; without optimisations: 0.022 s.
- ▶ Mathematica[®]: 0.017 s.

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Notes

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J. Aransay and J. Divasón. A formalisation in HOL of the Fundamental Theorem of Linear Algebra and its application to the solution of the least squares problem. *Journal of Automated Reasoning*. 2016

Judgment Day (iarrays and floating-point numbers for $\mathbb{R}$)

Comparison of the solutions to $H_6x = b$

- ▶ 1: Least squares approximation using rationals
- ▶ 2: *QR* approximation using floating-point numbers
- ▶ 3: Gauss-Jordan approximation using floating-point numbers

1 : -13824	415170	-2907240	7754040	-8724240	3489948
2 : -13824.0	415170.0001	-2907240.0	7754040.001	-8724240.001	3489948.0
3 : -13808.6421	414731.7866	-2904277.468	7746340.301	-8715747.432	3486603.907

Judgment Day

Size (n)	Poly/ML (s.)
100	0.88
200	10.88
300	84.40
400	184.11

Table : Elapsed time (in seconds) to compute the QR decomposition of H_n with floating-point precision



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J. Aransay and J. Divasón. *QR Decomposition*. Archive of Formal Proofs. 2015

Introduction

Gauss-Jordan

QR Decomposition

Conclusions

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- ▶ Linear Algebra algorithms can be implemented in HMA (linked to mathematical results)
- ▶ Algorithms are executable inside of Isabelle
- ▶ Better performance can be obtained thanks to code generation in SML and Haskell
- ▶ The use of immutable arrays does not pose a drawback, even in comparison to imperative programming

Further Work

- ▶ Explore the possibilities of optimization of rational numbers operations in SML

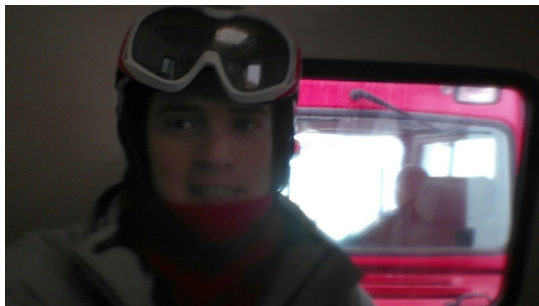
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- ▶ Explore the possibilities of optimization of rational numbers operations in SML
- ▶ Improve the ease to produce proofs of refinements
- ▶ Explore floating-point numbers possibilities

Good Luck!!!



thank you!