Real Vector Spaces, the Cauchy-Schwarz Inequality, & Convex Functions in ACL2(r)

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Introduction

Outline:

- Framework for reasoning about real vector spaces and convex functions
  - The Cauchy-Schwarz inequality
- Proof "engineering"
  - Design proofs such that theorem statements are clear and concise
  - Avoid fundamental logical limitations

Motivation:

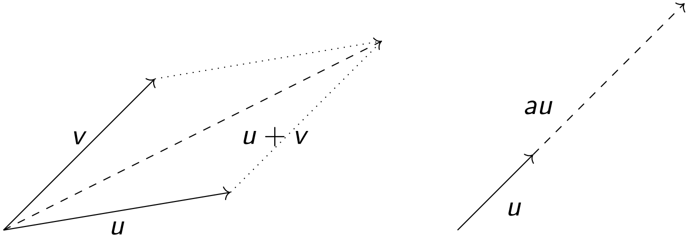
- Reasoning about convex optimisation algorithms
- Cauchy-Schwarz is useful and elegant
  - Top 100 Theorems / Formalising 100 Theorems[1]

[1] `cs.ru.nl/~freek/100`

Vector Spaces

$(\mathbb{R}^n, \mathbb{R}, \cdot, +)$ such that

- $+ : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is associative and commutative
- Identity elements: $0 + v = v$ and $1v = v$
- Inverse elements: $v + (-v) = 0$
- Compatibility: $a(bv) = (ab)v$
- Distributivity (two ways):
  $a(u + v) = au + uv$ and $(a + b)v = av + bv$



Inner Product Spaces

Inner Product Space = Vector Space + Inner Product
$\langle -, - \rangle : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$

- Positive-definiteness: $\langle u, u \rangle \geq 0$ and $\langle u, u \rangle = 0 \iff u = 0$
- Symmetry[2]: $\langle u, v \rangle = \langle v, u \rangle$
- Linearity of the first coordinate:
  $\langle au + v, w \rangle = a\langle u, w \rangle + \langle v, w \rangle$

For $\mathbb{R}^n$ and $u = (u_i)_{i=1}^n$, $v = (v_i)_{i=1}^n$, use the dot product:

$$\langle u, v \rangle = \sum_{i=1}^{n} u_i v_i$$

[2] when over $\mathbb{R}$

Cauchy-Schwarz

Theorem 1 (The Cauchy-Schwarz Inequality)

Let $u, v \in \mathbb{R}^n$. Then

$$|\langle u, v\rangle|^2 \leq \langle u, u\rangle\langle v, v\rangle \tag{CS1}$$

or, equivalently,

$$|\langle u, v\rangle| \leq \|u\| \cdot \|v\| \tag{CS2}$$

with equality iff u, v are linearly dependent. Here $\|u\| := \sqrt{\langle u, u\rangle}$.

How to prove it? Clever set-up + basic algebraic manipulations

Proof of $|\langle u, v\rangle|^2 \leq \langle u, u\rangle\langle v, v\rangle$

How to prove it? Clever set-up + basic algebraic manipulations:

Proof (sketch).

From positive-definiteness:

$$0 \leq \langle u - av, u - av\rangle = \langle u, u\rangle - 2a\langle u, v\rangle + a^2\langle v, v\rangle.$$

Set $a = \frac{\langle u,v\rangle}{\langle v,v\rangle}$ and rearrange (a bunch) to get

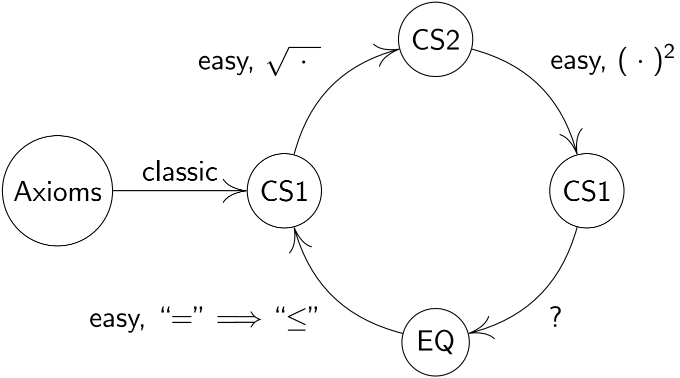
$$0 \underset{\uparrow}{\leq} \cdots \underset{\uparrow}{=} \langle u, u\rangle + \langle u, v\rangle \left(-2\frac{\langle u, v\rangle}{\langle v, v\rangle} + \frac{\langle u, v\rangle}{\langle v, v\rangle}\right) \underset{\uparrow}{=} \langle u, u\rangle - \frac{\langle u, v\rangle^2}{\langle v, v\rangle}.$$

$\square$

How to formalise it? Follow (mostly) from the classical proofs.

Structure of Cauchy-Schwarz

Approach:



CS1: $|\langle u, v\rangle|^2 \leq \langle u, u\rangle\langle v, v\rangle$ CS2: $|\langle u, v\rangle| \leq \|u\|\|v\|$

EQ: $|\langle u, v\rangle|^2 = \langle u, u\rangle\langle v, v\rangle \iff \exists a \in \mathbb{R},\ u = av$

Cauchy-Schwarz: Conditions for Equality

$$\begin{tikzcd} \text{EQ} & & \text{CS1} \arrow[ll] \end{tikzcd}$$

$\exists a \in \mathbb{R},\ u = av$

$|\langle u, v\rangle|^2 = \langle u, u\rangle\langle v, v\rangle$

In ACL2, just reverse and use positive-definiteness

$$0 \leq \langle u - av, u - av\rangle = \cdots = \langle u, u\rangle - \frac{\langle u, v\rangle^2}{\langle v, v\rangle}.$$

How to express "$\exists a$"?

1. Explicitly compute a from $|\langle u, v\rangle|^2 = \langle u, u\rangle\langle v, v\rangle$
   - hard & annoying
2. Use Skolem functions - much easier

Using Skolem Functions for Cauchy-Schwarz

Skolem functions have bodies with outermost quantifiers[3]:

```
(defun-sk linear-dependence (u v)
  (exists a (equal u (scalar-* a v))))
```

Requires a witness:

$$0 = \langle u - av, u - av \rangle \iff u - av = 0 \iff u = av$$

where $a = \frac{\langle u,v \rangle}{\langle v,v \rangle}$ from before.

[3] `scalar-*` is scalar-vector multiplication

Real Vector Spaces & Cauchy-Schwarz - Summary

Results:

- Reason about real vector & inner product spaces
- Formalised Cauchy-Schwarz inequality

Proof design issues:

- Exhibiting linear dependence in Cauchy-Schwarz
  - Use Skolem functions
  - Explicitly computing coefficients is hard
    - why compute when you don't need to?

Metric Spaces

$$\langle u - v, u - v \rangle = \|u - v\|^2 = d^2(u, v)$$

$$\text{inner products} \rightarrow \text{ norms } \longrightarrow \text{metrics}$$

(M, d) where $d : M \times M \rightarrow \mathbb{R}$ such that

1. Indiscernibility: $d(x, y) = 0 \iff x = y$
2. Symmetry: $d(x, y) = d(y, x)$
3. Triangle inequality: $d(x, y) \leq d(x, z) + d(z, y)$

Let $M = \mathbb{R}^n$ and $d(x, y) = \|x - y\|$:

1. & 2. Immediate

3. Use Cauchy-Schwarz: let $x = x' - z$, $y = z - y'$

$$\begin{aligned} \|x + y\|^2 &= \|x\|^2 + 2\langle x, y \rangle + \|y\|^2 \\ &\leq \|x\|^2 + 2\|x\|\|y\| + \|y\|^2 = (\|x\| + \|y\|)^2 \end{aligned}$$

Univariate/Multivariate Non-standard Analysis[4]

A number x is *standard* if it satisfies our usual definition of real.
A number $x > 0$ is *i-small* if it is less than any positive standard.

Continuity: A function f is *continuous* at a standard x if for any y

$$d(x, y) \text{ i-small} \implies d(f(x), f(y)) \text{ i-small}$$

Univariate	Multivariate
$f : \mathbb{R} \to \mathbb{R},\ d = \lvert \cdot \rvert$	$f : \mathbb{R}^n \to \mathbb{R},\ d = \lVert \cdot \rVert$

Differentiability: The *derivative* of f is a function f' satisfying the conditions below for "i-small" h

Univariate	Multivariate
$f'(x) = \frac{f(x+h)-f(x)}{h}$	$\frac{\lVert f(x+h)-f(x)-\langle f'(x),h\rangle \rVert}{\lVert h \rVert} = 0$

What does "i-small" mean for a vector in $\mathbb{R}^n$?

[4]informal

Recognizing "i-small" Vectors

Want:

```
(defun i-small-vecp (vec)
 (if (null vec) t (and (i-small (car vec))
                       (i-small-vecp (cdr vec)))))
```

NO! Non-classical[5] recursive functions are prohibited! Instead,

$$\|x\| = \sqrt{\sum_{i=1}^{n} z_i^2} \geq \max_i |x_i| \geq |x_i|$$

so

$$\|x\| \text{ i-small} \implies |x_i| \text{ i-small } \forall i \in [1, n]$$

[5] functions defined only in ACL2(r)

Recognizing "i-small" Vectors

$$\|x\| \text{ i-small} \implies |x_i| \text{ i-small } \forall i \in [1, n]$$

Avoid recursion by reasoning over i:

```
(defthm eu-norm-i-small-implies-elements-i-small
 (implies (and (real-listp x)
               (i-small (eu-norm x))
               (natp i)
               (< i (len x)))
          (i-small (nth i x))))
```

`eu-norm` is the Euclidean norm

Real Vector & Metric Spaces - Summary

Results:

- Reason about real vector spaces
- Reason about real metric spaces
  - Multivariate continuity & differentiability

Proof design issues:

- Exhibiting linear dependence in Cauchy-Schwarz
- Defining continuity
  - Non-classical recursive functions are prohibited
  - Show the largest entry in the vector is i-small
  - Reason about the index of arbitrary entries in the vector to avoid recursion

Convex Functions

A function $f : \mathbb{R}^n \to \mathbb{R}$ is *convex* if for all $\alpha \in [0, 1] \subset \mathbb{R}$, $x, y \in \mathbb{R}^n$

$$f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y).$$

Theorem 2

Let $f, g : \mathbb{R}^n \to \mathbb{R}$, $h : \mathbb{R} \to \mathbb{R}$ be convex. Then

1. $a \cdot f$ is convex for all $a \in \mathbb{R}_{\geq 0}$,
2. $f + g$ is convex,
3. $h \circ f$ is convex.

But how do we reason about functions?

Encapsulating Convex Functions

Encapsulate and suppress function definitions after proving hypotheses:

```
(encapsulate
 ...
 (local (defun cvfn-1 (x) ... 1337))
 ...
 (defthm cvfn-1-convex
  (implies ... ;; hypotheses
           (<= (cvfn-1 (vec-+ (scalar-* a x)
                              (scalar-* (- 1 a) y)))
               (+ (* a (cvfn-1 x))
                  (* (- 1 a) (cvfn-1 y))))) ...)

 (local (in-theory (disable cvfn-1)))

 ... ;; prove theorems about cvfn-1
 )
```

How do we reason about the convexity of a function?

Nesterov's Theorem

Theorem 3 (Nesterov)

"All the conditions below, holding for all $x, y \in \mathbb{R}^n$ and α from $[0, 1]$, are equivalent to inclusion $f \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$:"[6]

$$f(y) \leq f(x) + \langle f'(x), y - x \rangle + \frac{L}{2}\|x - y\|^2 \tag{N1}$$

$$f(x) + \langle f'(x), y - x \rangle + \frac{1}{2L}\|f'(x) - f'(y)\|^2 \leq f(y) \tag{N2}$$

$$\frac{1}{L}\|f'(x) - f'(y)\|^2 \leq \langle f'(x) - f'(y), x - y \rangle \tag{N3}$$

$$\langle f'(x) - f'(y), x - y \rangle \leq L\|x - y\|^2 \tag{N4}$$

$$f(\alpha x + (1 - \alpha)y) + \frac{\alpha(1 - \alpha)}{2L}\|f'(x) - f'(y)\|^2 \leq \alpha f(x) + (1 - \alpha)f(y) \tag{N5}$$

$$\alpha f(x) + (1 - \alpha)f(y) \leq f(\alpha x + (1 - \alpha)y) + \alpha(1 - \alpha)\frac{L}{2}\|x - y\|^2 \tag{N6}$$

[6] Yurii Nesterov's *Introductory Lectures on Convex Optimization*

Lipschitz Continuity

What is $\mathcal{F}_L^{1,1}(\mathbb{R}^n)$?

A function f belongs to the class $\mathcal{F}_L^{p,q}(\mathbb{R}^n)$, $p \geq q$, if

- f is p-times continuously differentiable on $\mathbb{R}^n$, ie. in $C^p(\mathbb{R}^n)$
- f is convex, ie. in $\mathcal{F}(\mathbb{R}^n)$
- the q-th derivative of f is L-Lipschitz continuous on $\mathbb{R}^n$, ie. $f^{(q)} \in C_L(\mathbb{R}^n)$

A derivative (gradient) f' of a function f is *L-Lipschitz continuous* if

$$\|f'(x) - f'(y)\| \leq L\|x - y\|$$

Ambiguities in Nesterov's Theorem

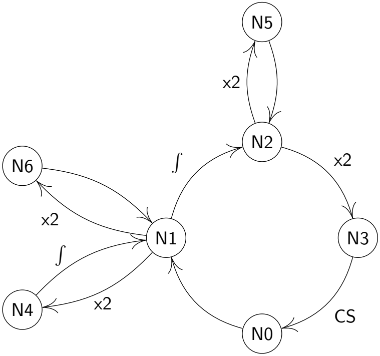
"All the conditions below, holding for all $x, y \in \mathbb{R}^n$ and α from $[0,1]$, are equivalent to inclusion $f \in \mathcal{F}_L^{1,1}(\mathbb{R}^n)$: ... [N1 - N6]"

What does Nesterov mean?

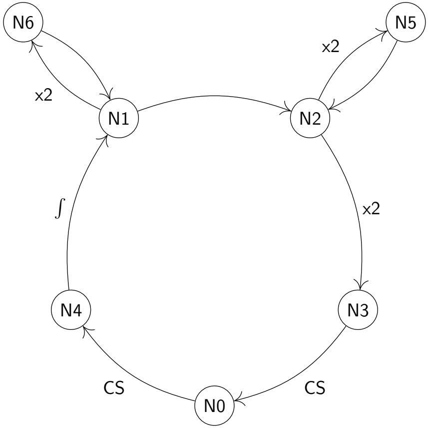
$\forall f : \mathbb{R}^n \to \mathbb{R},$	$f \in \mathcal{F}_L^{1,1} \iff \text{N1} \iff \cdots \iff \text{N6}$	False
$\forall f \in C,$	$f \in \mathcal{F}_L^{1,1} \iff \text{N1} \iff \cdots \iff \text{N6}$	False
$\forall f \in C^1,$	$f \in \mathcal{F}_L^{1,1} \iff \text{N1} \iff \cdots \iff \text{N6}$	False
$\forall f \in C^{1,1},$	$f \in \mathcal{F}_L^{1,1} \iff \text{N1} \iff \cdots \iff \text{N6}$	False
$\forall f \in \mathcal{C}_L^{1,1},$	$f \in \mathcal{F}_L^{1,1} \iff \text{N1} \iff \cdots \iff \text{N6}$	Almost True
$\forall f \in \mathcal{F}^{1,1},$	$f \in \mathcal{F}_L^{1,1} \iff \text{N1} \iff \cdots \iff \text{N6}$	True

Nesterov's Theorem in ACL2(r)

Nesterov's approach



Formalisation approach



CS: Cauchy-Schwarz $\int$: integration

N0: Lipschitz Continuity x2: instantiating inequalities twice

Instantiating Inequalities

Sometimes we need to add two "copies" of an inequality, eg. two copies of N2 with variables swapped give N3

$$
\begin{aligned}
f(x) + \langle f'(x), y - x \rangle + \frac{1}{2L}\|f'(x) - f'(y)\|^2 &\leq f(y), \\
f(y) + \langle f'(y), x - y \rangle + \frac{1}{2L}\|f'(y) - f'(x)\|^2 &\leq f(x), \\
\implies \frac{1}{L}\|f'(x) - f'(y)\|^2 &\leq \langle f'(x) - f'(y), x - y \rangle
\end{aligned}
$$

Usually,

```
(defthm ineq-N2-implies-ineq-N3
 (implies (and (real-listp x) (real-listp y) ...
               (ineq-N2 x y))
          (ineq-N3 x y)))
```

How do we instantiate N2 with swapped variables?

Instantiating Inequalities

Maybe:

```
(implies (ineq-N2 x y) (ineq-N2 y x))
```

But this is not (necessarily) true:

$$\forall x, y, (P(x, y) \implies P(y, x))$$

What Nesterov means is:

$$(\forall x, y, P(x, y)) \implies (\forall x, y, P(y, x)) \qquad (*)$$

Maybe:

```
(implies (and ... (ineq-N2 x y) (ineq-N2 y x))
         (ineq-N3))
```

But then N1 $\implies$ N2 would need two copies of N1, too! Etc.
Stronger than $(*)$ but messy.

Instantiating Inequalities

Use Skolem functions (again), eg.[7]

```
(defun-sk ineq-N2-sk ...
 (forall (x y) (ineq-N2 x y)))
```

Instantiate as needed, eg.

```
(implies (ineq-N2-sk ...)
         (and (ineq-N2 x y) (ineq-N2 y x)))
```

[7] slightly more complicated in reality

Nesterov's Final Form

$$\text{N0} \iff \text{N1} \iff \cdots \iff \text{N6}$$

means

$$(\text{N0} \vee \text{N1} \vee \cdots \vee \text{N6}) \implies (\text{N0} \wedge \text{N1} \wedge \cdots \wedge \text{N6})$$

If any one is true, we get the rest for free, eg.

```
(defthm nesterov
 (implies (or (ineq-N0 ...) (ineq-N1 ...) ...)
          (and (ineq-N0 ...) (ineq-N1 ...) ...)))
```

Conclusion

We saw

- A new framework for reasoning about real vector spaces and convex functions
  - A formal first-order proof of the Cauchy-Schwarz inequality
- Proof "engineering": design proofs so that
  - theorem statements are clean and unambiguous
  - fundamental logical limitations are avoided

Future:

- Convex optimisation and machine learning algorithms
  - eg. Stochastic gradient descent, perceptron, etc.
- Multivariate analysis
- Generalisations of vector/metric spaces
  - eg. Abstract inner product spaces, Hilbert spaces, etc.

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Thank You