Formally Verified Approximations of Definite Integrals

Assia Mahboubi Guillaume Melquiond
Thomas Sibut-Pinote

Inria & LRI, Université Paris Sud, CNRS

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Numerical Integrals in Modern Math Proofs

Double bubbles minimize

The proof parameterizes the space of possible solutions by a two-dimensional rectangle [...]. This rectangle is subdivided into 15,016 smaller rectangles which are investigated by calculations involving a total of 51,256 numerical integrals.

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Major arcs for Goldbach's problem

$$\int_{-\infty}^{\infty} \frac{(0.5 \cdot \log(\tau^2 + 2.25) + 4.1396 + \log \pi)^2}{0.25 + \tau^2} d\tau$$

We compute the last integral numerically (from -100,000 to 100,000).

mathoverflow

Questions Tags Users Badges Una

Rigorous numerical integration

9

2

I need to evaluate some (one-variable) integrals that neither SAGE nor Mathematica can do symbolically. As far as I can tell, I have two options:

(a) Use GSL (via SAGE), Maxima or Mathematica to do numerical integration. This is really a non-option, since, if I understand correctly, the "error bound" they give is not really a guarantee.

(b) Cobble together my own programs using the trapezoidal rule, Simpson's rule, etc., and get rigorous error bounds using bounds I have for the second (or fourth, or what have you) derivative of the function I am integrating. This is what I have been doing.

Is there a third option? Is there standard software that does (b) for me?

na.numerical-analysis

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asked Mar 5 '13 at 23:03

H A Helfgott

3,141 • 17 • 61

Introduction

Objective

A tool for computing guaranteed bounds on definite integrals.

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Methodology

- define a robust yet efficient algorithm,
- formally prove that it is correct,
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Bonus objective

A tool for proving that a function is integrable on a domain.

Outline

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Coq: a Proof Assistant

Support

- typed lambda-calculus with inductive types,
- proof verification using a “small” kernel,
- proof assistance using tactic-based backward reasoning.

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Stating and proving $\frac{ab}{ac} = \frac{b}{c}$

```
Lemma Rdiv_compat_r : (* stating the theorem *)
  forall a b c : R,
  a <> 0 -> c <> 0 -> (a*b) / (a*c) = b/c.
Proof. (* building the proof using tactics *)
  intros.
  field.
  easy.
Qed. (* verifying the resulting proof *)
```

Automatic Proof using CoqInterval

Support

Quantifier-free formulas of enclosures of expressions using

- basic arithmetic operators: $+$, $-$, $\times$, $\div$, $\sqrt{\cdot}$,
- elementary functions: cos, sin, tan, arctan, exp, log.

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Approach

Fully formalized in Coq:

- efficient multi-precision FP arithmetic,
- interval arithmetic with univariate Taylor models,
- reflexive tactic.

Automatic Proof using CoqInterval

Stating and proving $x \leq 3 \Rightarrow \sqrt{\exp x} <= 5$

```
Lemma whatever :
  forall x : R, x <= 3 -> sqrt (exp x) <= 5.
Proof.
  intros.
  interval.
Qed.
```

Outline

Interval Arithmetic

Definition (Interval)

An interval $\mathbf{x} \in \mathbb{I}$ is a closed subset of $\mathbb{R}$.

It is represented by floating-point bounds $[\underline{x}, \overline{x}]$ with $\underline{x} \in \mathbb{F} \cup \{-\infty\}$ and $\overline{x} \in \mathbb{F} \cup \{+\infty\}$.

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Definition (Interval extension)

For any function $f : \mathbb{R}^n \to \mathbb{R}$,
a function $F : \mathbb{I}^n \to \mathbb{I}$ is an *interval extension* of f on $\mathbb{R}$ if

$$\forall \mathbf{x}_1, \ldots, \mathbf{x}_n,\ \{f(x_1, \ldots, x_n) \mid \forall i, x_i \in \mathbf{x}_i\} \subseteq \mathbf{f}(\mathbf{x}_1, \ldots, \mathbf{x}_n).$$

Interval Arithmetic

Good points

Interval extensions can be computed cheaply by composition of simple operators:

- $[\underline{u}, \overline{u}] + [\underline{v}, \overline{v}] = [\triangledown(\underline{u} + \underline{v}), \triangle(\overline{u} + \overline{v})]$
- $[\underline{u}, \overline{u}] - [\underline{v}, \overline{v}] = [\triangledown(\underline{u} - \overline{v}), \triangle(\overline{u} - \underline{v})]$

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Bad points

When created that way, interval extensions compute overestimated enclosures if there are multiple occurrences of variables:

for $x \in [-1, 1]$, $\sin x - x \in [-0.2; 0.2]$, but $\sin \mathbf{x} - \mathbf{x} \subseteq [-1.9; 1.9]$.

Naive Integral Enclosure

Lemma (Naive integral enclosure)

For any intervals $\mathbf{u}, \mathbf{v}$ *such that* $u \in \mathbf{u}$ *and* $v \in \mathbf{v}$, *we have*

$$\int_u^v f(t)\,dt \in (\mathbf{v} - \mathbf{u}) \cdot \mathbf{f}(\mathbf{u} \cup \mathbf{v}).$$

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Example and splitting

$$\int_0^1 t\,dt \quad \in \quad (1 - 0) \cdot [0; 1] = [0; 1]$$

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Rule of thumb

Doubling the computation time increases the accuracy by one bit.

Polynomial Integral Enclosure

Lemma (Polynomial integral enclosure)

Suppose f *is approximated on* $[u, v]$ *by* $p \in \mathbb{R}[X]$ *and* $\mathbf{\Delta} \in \mathbb{I}$ *in the sense that* $\forall x \in [u, v],\ f(x) - p(x) \in \mathbf{\Delta}$*.*
Then for any primitive P *of* p

$$\int_u^v f(t)\,dt \in P(\mathbf{v}) - P(\mathbf{u}) + (\mathbf{v} - \mathbf{u}) \cdot \mathbf{\Delta}.$$

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Obtaining rigorous polynomial approximations

- Compute truncated Taylor series for transcendental functions.
- Combine polynomial approximations,
  e.g. $(P_1, \mathbf{\Delta_1}) + (P_2, \mathbf{\Delta_2}) = (P_1 + P_2, \mathbf{\Delta_1} + \mathbf{\Delta_2})$.

Adaptive Splitting

Computing an integral enclosure at a given accuracy

Inputs: interval $[u, v]$, target width δ.
Output: enclosure of $\int_u^v f$ of width at most δ.

Let m be the midpoint of $[u, v]$.
Let $\mathbf{i}_1$ and $\mathbf{i}_2$ be enclosures of $\int_u^m f$ and $\int_m^v f$.

If $w(\mathbf{i}_1 + \mathbf{i}_2) > \delta$,

- if $w(\mathbf{i}_1) \leq \delta/2$,
  - recompute $\mathbf{i}_2$ recursively using $[m, v]$ and $\delta - w(\mathbf{i}_1)$,
- if $w(\mathbf{i}_2) \leq \delta/2$,
  - recompute $\mathbf{i}_1$ recursively using $[u, m]$ and $\delta - w(\mathbf{i}_2)$,
- otherwise recompute recursively both $\mathbf{i}_1$ and $\mathbf{i}_2$ using $\delta/2$.

Return $\mathbf{i}_1 + \mathbf{i}_2$.

Integrability

Lemma (Naive integral enclosure)

For any intervals $\mathbf{u}, \mathbf{v}$ such that $u \in \mathbf{u}$ and $v \in \mathbf{v}$,
if f is integrable between u and v, $\int_u^v f(t)\,dt \in (\mathbf{v} - \mathbf{u}) \cdot \mathbf{f}(\mathbf{u} \cup \mathbf{v})$.

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Lemma (Naive integral enclosure and integrability)

For any intervals $\mathbf{u}, \mathbf{v}$ such that $u \in \mathbf{u}$ and $v \in \mathbf{v}$,
if $(\mathbf{v} - \mathbf{u}) \cdot \mathbf{f}(\mathbf{u} \cup \mathbf{v})$ evaluates to an interval $\mathbf{i}$,
then f is integrable on $[u, v]$, and $\int_u^v f(t)\,dt \in \mathbf{i}$.

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Trick

When computed by CoqInterval, $\mathbf{f}$ has the following property:

$\mathbf{f}(\mathbf{x})$ evaluates to an intvl only if f is defined and continuous on $\mathbf{x}$.

Outline

1. Introduction
2. Numerical enclosures of integrals
3. Examples
   - Demo
   - Comparison to other tools
   - Helfgott's integral on MathOverflow
   - Rump's integral in Tucker's book
4. Conclusion

Demo

$$\int_0^1 \sqrt{1 - x^2}\, dx = \frac{\pi}{4}$$

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```
Lemma quarter_disk :
  Rabs (RInt (fun x => sqrt(1 - x * x)) 0 1 - PI/4) <=
       1/10^9.
Proof.
interval with (i_prec 40, (* FP precision: 40 bits *)
  i_integral_prec 30,  (* target accuracy: 30 bits *)
  i_integral_depth 20, (* maximal depth *)
  i_integral_deg 10).  (* degree of pol approx *)
Qed. (* proof time: 2 seconds *)
```

Comparison to Other Tools

- Matlab/Octave: numerical quadrature, `quad` (Gauss), `quadv` (Simpson), `quadcc` (Clenshaw-Curtis), `quadgk` (Gauss-Kronrod), `quadl` (Lobatto).
- Intlab: reliable quadrature using Taylor models.
- VNODE-LP: reliable ODE solver using Taylor models.

Non-Smooth Integrand

Example (Helfgott's integral on MathOverflow)

$$\int_0^1 \left|\left(x^4 + 10x^3 + 19x^2 - 6x - 6\right) \exp x\right| dx$$

Results when asked for 15 correct digits

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- VNODE-LP: absolute value not supported. ✧

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Results using CoqInterval

Target	Time	Degree	Depth	Prec
10^{-3}	0.7	5	8	30
10^{-6}	0.9	6	13	40
10^{-9}	1.3	8	18	50
10^{-12}	1.9	10	22	60
10^{-15}	2.7	12	28	70

Oscillating Integrand

Example (Rump's integral in Tucker's book)

$$\int_0^8 \sin(x + \exp x)\, dx$$

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Target	Time	Degree	Depth	Prec
10^{-1}	81.0	6	12	30
10^{-2}	123.6	8	12	30
10^{-3}	183.4	10	12	30
10^{-4}	277.6	12	12	30

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High accuracy is still out of range on such an example.

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Conclusion and Perspectives

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`http://coq-interval.gforge.inria.fr/`