Adaptive quadratures work well even for piecewise smooth functions(?)

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The problem

For

$$f : [a, b] \to \mathbb{R}$$

compute (numerically)

$$I(a, b; f) = \int_a^b f(x)\,\mathrm{d}x$$

using a finite number of evaluations of f, i.e.,

$$Q_n(f) = \varphi_n\big(f(x_1), f(x_2), \ldots, f(x_n)\big).$$

If x_i depends on $f(x_1), \ldots, f(x_{i-1})$ then the approximation is adaptive.

A generally accepted tool:

ADAPTIVE QUADRATURES.

Adaptive quadratures

Generic idea:

1. Two “simple” quadrature rules, $S_1(a,b;f)$ and $S_2(a,b;f)$, are computed for $I(a,b;f)$.
2. If the difference $|S_1(a,b;f) - S_2(a,b;f)|$ is “small enough” then the calculations terminate and $I(a,b;f)$ is approximated by $S_2(a,b;f)$.
3. Otherwise the interval $[a,b]$ is divided into two (or more) equal length subintervals, and the same rule is applied recursively to each of the subintervals.

Adaptive quadratures are used for automatic integration within ε.

Questions

1. For which functions adaptive quadratures work well?
2. What is the best subdivision strategy?

A common knowledge is that:

Adaptive quadratures work well for integration of sufficiently smooth functions, but usually fail for integration of piecewise smooth functions.

This is not quite true!

We give more accurate answers taking as an example

ADAPTIVE SIMPSON QUADRATURES.

Standard Simpson quadrature

For a subinterval $[u, v]$ with $h = v - u > 0$

$$\begin{aligned} S_1(u,v;f) &= \frac{h}{6}\left(f(u) + 4f\left(\frac{u+v}{2}\right) + f(v)\right), \\ S_2(u,v;f) &= S_1\left(u, \frac{u+v}{2}; f\right) + S_1\left(\frac{u+v}{2}, v; f\right). \end{aligned}$$

<u>Standard</u> adaptive quadrature:

function $Q = \mathrm{STD}(f, a, b, \varepsilon)$
  $S1 = S_1(a,b;f);\ S2 = S_2(a,b;f);$
  if $|S1 - S2| \leq 15\,\varepsilon$
    $Q = S2;$
  else
    $Q = \mathrm{STD}\left(f, a, \frac{a+b}{2}, \frac{\varepsilon}{2}\right) + \mathrm{STD}\left(f, \frac{a+b}{2}, b, \frac{\varepsilon}{2}\right);$
  end if
end function

Why does it work?

Let $f \in C^4([a,b])$. For $s \in [u,v]$ with $f^{(4)}(s) \neq 0$ use (well known)

$$S_1(u,v;f) - S_2(u,v;f) \approx 15\left(S_2(u,v;f) - I(u,v;f)\right), \quad \text{as} \quad h \to 0.$$

Since STD terminates for $[u,v]$ when $|S1 - S2| \leq 15\,\varepsilon\, h/(b-a)$, the total error is

$$\lessapprox \sum_{i=1}^{m} \frac{h_i}{b-a}\varepsilon = \varepsilon,$$

provided $f^{(4)} > 0$.

The (non-asymptotic!) inequality *(P. 2015)*

$$0 \leq S_2(u,v;f) - I(u,v;f) \leq S_1(u,v;f) - S_2(u,v;f)$$

allows to extend this result to $f^{(4)} \geq 0$.

Optimal Simpson quadrature

Optimal adaptive quadrature *(P. 2015)*:

function $Q = \mathrm{OPT}(f, a, b, \hat{\varepsilon})$
  $S1 = S_1(a,b;f)$; $S2 = S_2(a,b;f)$;
  if $|S1 - S2| \leq 15\,\hat{\varepsilon}$
    $Q = S2$;
  else
    $Q = \mathrm{OPT}\left(f, a, \frac{a+b}{2}, \hat{\varepsilon}\right) + \mathrm{OPT}\left(f, \frac{a+b}{2}, b, \hat{\varepsilon}\right)$;
  end if
end function

OPT is run with $\hat{\varepsilon} = \varepsilon$ obtaining an "in between" partition consisting of m_1 subintervals. Then OPT is resumed with the updated value $\hat{\varepsilon} = \varepsilon_1$, where

$$\varepsilon_1 = \varepsilon\, m_1^{-5/4}.$$

Asymptotic error

Let $Q_m^{\text{opt}}(a,b;f)$ and $Q_m^{\text{std}}(a,b;f)$ be the results returned by OPT and STD, where m is the number of subintervals in the final partition. Let

$$Z = \{\, x \in (a,b) : f^{(4)}(x) \neq 0 \,\}$$

Theorem (*P. 2015, Kałuża & P. 2024*)

Let $f \in C^4([a,b])$ *with* $f^{(4)} \geq 0$. *Then*

$$\begin{aligned} Q_m^{\text{opt}}(a,b;f) - I(a,b;f) &= \kappa_{\text{opt}}(m)\gamma \left\| f^{(4)} \right\|_{L^{1/5}(Z)} m^{-4}, \\ Q_m^{\text{std}}(a,b;f) - I(a,b;f) &= \kappa_{\text{std}}(m)\gamma \, |Z| \left\| f^{(4)} \right\|_{L^{1/4}(Z)} m^{-4}, \end{aligned}$$

where $\gamma = \frac{1}{2^4 \times 2880} \cong 2.17 \times 10^{-5}$ *and*

$$1 \lessapprox \kappa_{\text{opt}}(m) \lessapprox K_{\text{opt}} \cong 2.8954, \qquad \kappa_{\text{std}}(m) \lessapprox K_{\text{std}} = 16.$$

Effectiveness of the adaptive quadratures

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Theorem (*P. 2015, Kałuża & P. 2024*)

Suppose $f \in C^4([a,b])$ *with* $f^{(4)} \geq 0$.
For given error demand ε*, the quadratures* STD *and* OPT *return an approximation to the integral* $I(a,b;f)$ *with error that* *asymptotically* *(as* $\varepsilon \to 0^+$*) is at most* ε*.*

Piecewise smooth functions

$$f(x) = g(x) + \sum_{l=1}^{\nu} \sum_{k=0}^{4} \Delta_{k,l}\, \phi_k(x, s_l), \qquad \phi_k(x, s_l) = \frac{(x - s_l)_+^k}{k!},$$

where $g \in C^4([a,b])$ is the smooth part, s_l are singular points, and $\Delta_{k,l}$ are discontinuity jumps

$$\Delta_{k,l} = f^{(k)}(s_l^+) - f^{(k)}(s_l^-), \qquad 0 \le k \le 4, \quad 1 \le l \le \nu.$$

For instance, if $f(x) = |\cos(x)|$ with $x \in [0, 5]$ then

$$\begin{aligned} g(x) &= |\cos(x)| - 2\left((x - \pi/2)_+ + (x - 3\pi/2)_+\right) \\ &\quad + \frac{1}{3}\left((x - \pi/2)_+^3 + (x - 3\pi/2)_+^3\right). \end{aligned}$$

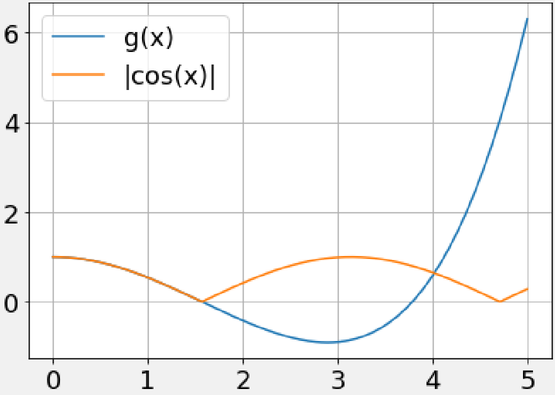

Figure: The function $|\cos(x)|$ and its smooth part $g(x)$.

A numerical example

Test 1: (discontinuous functions)

$$[a, b] = [0, 1], \quad \nu = 13, \quad \Delta_{4,l} = 0, \quad g(x) = \frac{1}{x + 10^{-5}}.$$

All the other parameters are random and mutually independent;

$$s_l \sim \mathcal{U}(0, 1), \qquad \Delta_{k,l} \sim \mathcal{N}\left(0, (k + l)^2\right).$$

STD fails for discontinuous functions!

$-\log(\varepsilon)$	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	5.5	6.0	6.5	7.0	7.5	8.0
OPT	34%	31%	12%	5%	1%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%

Table: Percentage of failures for given ε: discontinuous case.

Test 2: (continuous functions)

It differs from Test 1 by $\Delta_{0,l} = 0$, with the other parameters unchanged.

$-\log(\varepsilon)$	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	5.5	6.0	6.5	7.0	7.5	8.0
STD	0%	12%	41%	39%	47%	45%	39%	20%	11%	8%	7%	4%	1%	0%	0%
OPT	0%	3%	5%	11%	8%	9%	6%	5%	2%	1%	1%	0%	0%	0%	0%

Table: Percentage of failures for given ε: continuous case.

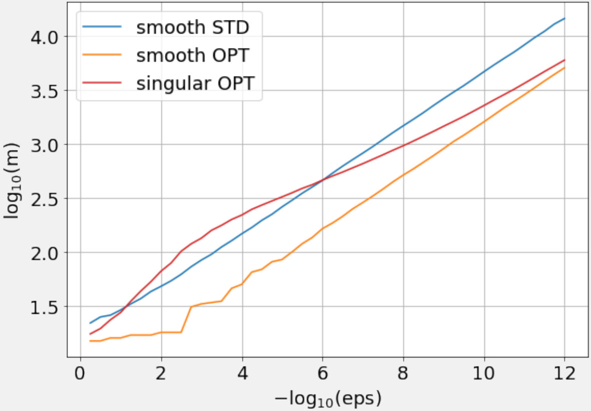

Figure: Smooth vs. singular functions: discontinuous case

STD fails for discontinuous functions!

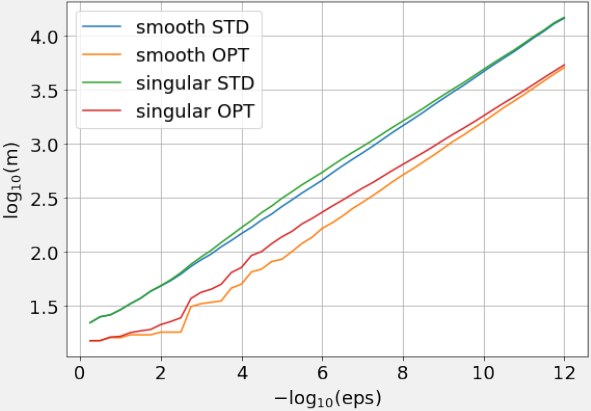

Figure: Smooth vs. singular functions: continuous case

So good? Why?

Questions:

(i) how big is the local error $|S_2(u,v;f) - I(u,v;f)|$, and

(ii) how well is $|S_2(u,v;f) - I(u,v;f)|$ estimated by $|S_1(u,v;f) - S_2(u,v;f)|$,

in subintervals $[u,v)$ containing singularities?

Example:

Let $g = 0,\ \nu = 1,\ s = 0.8,$ and

$$(\Delta_0, \Delta_1, \Delta_2, \Delta_3, \Delta_4) = (-9991, 1, -1, 1, 0).$$

Then

$$\begin{aligned} S_1(0,1;f) - S_2(0,1;f) &\cong 0.07105 \\ S_2(0,1;f) - I(0,1;f) &\cong -1988.97 \end{aligned}$$

But this may happen only in 'exceptional' cases (!)

Main result

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We consider

$$f(x) = g(x) + \sum_{l=1}^{\nu} \sum_{k=0}^{4} \Delta_{k,l}\, \phi_k(x, s_l), \qquad \phi_k(x, s_l) = \frac{(x - s_l)_+^k}{k!},$$

where g and ν are given and the remaining parameters

$$\mathcal{T} = (s_j, \Delta_{0,j}, \Delta_{1,j}, \Delta_{2,j}, \Delta_{3,j}, \Delta_{4,j})_{j=1}^{\nu}$$

are random variables distributed according to a probability measure μ on $\Omega = \big([a, b) \times \mathbb{R}^5\big)^{\nu}$.

Main result

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Theorem (*Kałuża & P. 2024*)

Suppose the piecewise smooth function f is a realization of the random process governed by a probability measure μ, such that $f^{(4)} \geq 0$ μ-a.s. If μ is absolutely continuous then with probability 1 *we have*

$$Q_m^{\mathrm{opt}}(a,b;f) - I(a,b;f) = \kappa_{\mathrm{opt}}(m)\,\gamma\,\left\|f^{(4)}\right\|_{L^{1/5}(Z)} m^{-4},$$

where $1 \lessapprox \kappa_{\mathrm{opt}}(m) \lessapprox K_{\mathrm{opt}} \cong 2.8954.$
If, in addition, f is continuous μ-a.s. then with probability 1

$$Q_m^{\mathrm{std}}(a,b;f) - I(a,b;f) = \kappa_{\mathrm{std}}(m)\,\gamma\,|Z|\,\left\|f^{(4)}\right\|_{L^{1/4}(Z)} m^{-4},$$

where $\kappa_{\mathrm{std}}(m) \lessapprox K_{\mathrm{std}} = 16.$

Justification

Let $s \in [u_n, v_n)$ be a singular point, $h_n = (b-a)/2^n$. Let

$$t_n = \frac{s - u_n}{v_n - u_n} \in [0, 1).$$

Then t_n evolves according to the dynamical system

$$t_n \; = \; 2\, t_{n-1} \bmod 1, \qquad n = 1, 2, 3.$$

An analysis of $\{t_n\}_{n \geq 0}$ shows that the following holds almost surely:

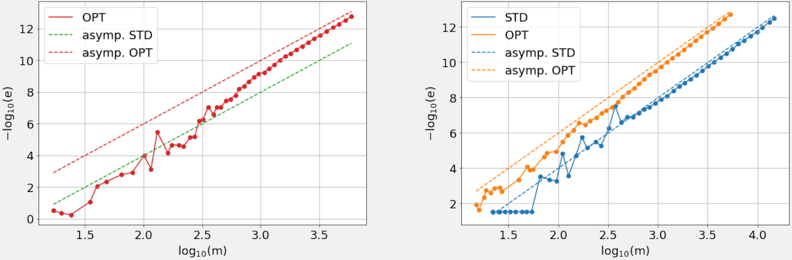
(i) $|S_1(u_n, v_n; f) - S_2(u_n, v_n; f)|$ is of order h_n if f is discontinuous at s, and of order h_n^2 otherwise,

(ii)

$$|S_2(u_n, v_n; f) - I(u_n, v_n; f)| \; \lessapprox \; K\, |S_1(u_n, v_n; f) - S_2(u_n, v_n; f)|$$

where $K = 2$ if f is discontinuous at s, and $K = 1$ otherwise.

A numerical example



(a) Discontinuous f (b) Continuous f

Figure: Optimal and standard quadratures for rapidly changing $f^{(4)}$.

Conclusion

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Corollary (*Kałuża & P. 2024*)

Suppose the measure μ on the set of piecewise smooth functions satisfies the assumptions of the Main Theorem.

Then μ-almost surely the quadratures STD *and* OPT *return approximations to $I(a,b;f)$ with error that asymptotically is at most ε.*

What if $f^{(4)}$ changes its sign?

Then the adaptive quadratures may fail; e.g., for

$$f(x) = \prod_{k=0}^{4} (x-k)^2, \qquad x \in [0,4].$$

If ”nothing but happens” and the quadratures produce “perfect partition”, the asymptotic factors depend on f via

$$\mathcal{L}^{\mathrm{opt}}(f) = \left(\|f^{(4)}\|_{L^{1/5}(Z_+)}^{1/5} - \|f^{(4)}\|_{L^{1/5}(Z_-)}^{1/5} \right) \|f^{(4)}\|_{L^{1/5}(Z_+ \cup Z_-)}^{4/5}$$

$$\mathcal{L}^{\mathrm{std}}(f) = \big(|Z_+| - |Z_-| \big) \|f^{(4)}\|_{L^{1/4}(Z_+ \cup Z_-)}$$

where

$$Z_+ \{x \in (a,b) : f^{(4)}(x) > 0\}, \qquad Z_- \{x \in (a,b) : f^{(4)}(x) < 0\}.$$

(Kałuża & P. 2024)

The actual errors are usually overestimated!

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