

The algorithms used in this section on integration and the next section on function recovery are all based on quadratic splines on $[0, 1]$. The node set and the quadratic spline algorithm using n function values are defined for $n \in \mathcal{I} := \{3, 5, 7, \dots\}$ as follows:

$$x_i = \frac{i-1}{n-1}, \quad i = 1, \dots, n, \quad (1a)$$

$$\begin{aligned} A_n(f)(x) := & \frac{(n-1)^2}{2} [f(x_i)(x-x_{i+1})(x-x_{i+2}) \\ & - 2f(x_{i+1})(x-x_i)(x-x_{i+2}) + f(x_{i+2})(x-x_i)(x-x_{i+1})] \\ & \text{for } x_i \leq x \leq x_{i+2}. \end{aligned} \quad (1b)$$

The cost of each function value is one and so the cost of A_n is n . The algorithm A_n is imbedded in the algorithm A_{3n-2} , which uses $3n-3$ subintervals. Thus, $r=3$ is the cost multiple.

The problem to be solved is univariate integration on the unit interval, $S(f) := \text{INT}(f) := \int_0^1 f(x) dx \in \mathcal{G} := \mathbb{R}$. The fixed cost building blocks to construct the adaptive integration algorithm are the composite Simpson's rules based on $n-1$ intervals:

$$\begin{aligned} P_n(f) &:= \int_0^1 A_n(f) dx \\ &= \frac{1}{3n-3} [f(x_1) + 4f(x_2) + 2f(x_3) + 4f(x_4) + 2f(x_5) \cdots + 4f(x_{n-1}) + f(x_n)]. \end{aligned} \quad (2)$$

The space of input functions is $\mathcal{F} := \mathcal{V}^3$, the space of functions whose third derivatives have finite variation. The general definitions of some relevant norms and spaces are as follows:

$$\text{Var}(f) := \sup_{\substack{n \in \mathbb{N} \\ 0=x_0 < x_1 < \dots < x_n=1}} \sum_{i=1}^n |f(x_i) - f(x_{i-1})|, \quad (3a)$$

$$\|f\|_p := \begin{cases} \left[\int_0^1 |f(x)|^p dx \right]^{1/p}, & 1 \leq p < \infty, \\ \sup_{0 \leq x \leq 1} |f(x)|, & p = \infty, \end{cases} \quad (3b)$$

$$\mathcal{V}^k := \mathcal{V}^k[0, 1] = \{f \in C[0, 1] : \text{Var}(f^{(k)}) < \infty\}, \quad (3c)$$

$$\mathcal{W}^{k,p} = \mathcal{W}^{k,p}[0, 1] = \{f \in C[0, 1] : \|f^{(k)}\|_p < \infty\}. \quad (3d)$$

The stronger semi-norm is $|f|_{\mathcal{F}} := \text{Var}(f''')$, while the weaker semi-norm is

$$|f|_{\tilde{\mathcal{F}}} := \|f'' - A_3(f)''\|_1 = \|f'' - 4[f(1) - 2f(1/2) + f(0)]\|_1 = \text{Var}(f' - A_3(f)'),$$

where $A_3(f) : x \mapsto 2f(0)(x - 1/2)(x - 1) - 4f(1/2)x(x - 1) + 2f(1)x(x - 1/2)$ is the quadratic interpolant of f using the middle point and two endpoints of the integration interval. The reason for defining $|f|_{\tilde{\mathcal{F}}}$ this way is that $|f|_{\tilde{\mathcal{F}}}$ vanishes if f is a quadratic function, and quadratic functions are integrated exactly by the Simpson's rule. The cone of integrands is defined as

$$\mathcal{C}_\tau := \left\{ f \in \mathcal{V}^3 : \begin{cases} \text{Var}(f''') \leq \tau \text{Var}(f'') \\ \text{Var}(f'') \leq \tau \|f'' - 4[f(1) - 2f(1/2) + f(0)]\|_1 \end{cases} \right\}. \quad (4)$$

The algorithm for approximating $\|f'' - 4[f(1) - 2f(1/2) + f(0)]\|_1$ is the $\tilde{\mathcal{F}}$ -semi-norm of the quadratic spline, $A_n(f)$:

$$\begin{aligned} \tilde{F}_n(f) &:= |A_n(f)|_{\tilde{\mathcal{F}}} = \|A_n(f)'' - A_3(f)''\|_1 \\ &= \sum_{j=1}^{(n-1)/2} \int_{x_{2j-1}}^{x_{2j+1}} |A_n(f)'' - A_3(f)''| \, dx, \\ &= \sum_{j=1}^{(n-1)/2} \int_{x_{2j-1}}^{x_{2j+1}} |(n-1)^2(f(x_{2j+1}) - 2f(x_{2j}) + f(x_{2j-1})) - 4[f(1) - 2f(1/2) + f(0)]| \, dx, \\ &= \sum_{j=1}^{(n-1)/2} |(n-1)^2(f(x_{2j+1}) - 2f(x_{2j}) + f(x_{2j-1})) - 4[f(1) - 2f(1/2) + f(0)]| (x_{2j+1} - x_{2j-1}), \\ &= \sum_{j=1}^{(n-1)/2} |(n-1)^2(f(x_{2j+1}) - 2f(x_{2j}) + f(x_{2j-1})) - 4[f(1) - 2f(1/2) + f(0)]| \frac{2}{n-1}, \\ &= \sum_{j=1}^{(n-1)/2} \left| 2(n-1)(f(x_{2j+1}) - 2f(x_{2j}) + f(x_{2j-1})) - \frac{8}{n-1}[f(1) - 2f(1/2) + f(0)] \right|. \end{aligned} \quad (5)$$

The variation of the second derivative of the quadratic spline of f , i.e.,

$$F_n(f) := \text{Var}(A_n(f)''') = (n-1)^2 \sum_{j=1}^{(n-3)/2} |f(x_{2j+3}) - 2f(x_{2j+2}) + 2f(x_{2j}) - f(x_{2j-1})|, \quad (6)$$

provides a lower bound on $\text{Var}(f')$ for $n \geq 5$.

Constructing the adaptive algorithm for integration requires an upper bound on the error of P_n and a two-sided bound on the error of \tilde{F}_n . Note that $\tilde{F}_n(f)$ never overestimates $|f|_{\tilde{\mathcal{F}}}$ because

$$\begin{aligned} |f|_{\tilde{\mathcal{F}}} &= \|f'' - A_3(f)''\|_1 = \sum_{j=1}^{(n-1)/2} \int_{x_{2j-1}}^{x_{2j+1}} |f''(x) - A_3(f)''(x)| \, dx \\ &\geq \sum_{j=1}^{(n-1)/2} \left| \int_{x_{2j-1}}^{x_{2j+1}} [f''(x) - A_3(f)''(x)] \, dx \right| = \|A_n(f)'' - A_3(f)''\|_1 = \tilde{F}_n(f). \end{aligned}$$

Thus, $h_-(n) := 0$ and $\mathbf{c}_n = \tilde{\mathbf{c}}_n = 1$.

To find an upper bound on $|f|_{\tilde{\mathcal{F}}} - \tilde{F}_n(f)$, note that

$$|f|_{\tilde{\mathcal{F}}} - \tilde{F}_n(f) = |f|_{\tilde{\mathcal{F}}} - |A_n(f)|_{\tilde{\mathcal{F}}} \leq |f - A_n(f)|_{\tilde{\mathcal{F}}} = \|f'' - A_n(f)''\|_1,$$

since $(f - A_n(f))(x)$ vanishes for $x = 0, 0.5, 1$. Moreover,

$$\|f'' - A_n(f)''\|_1 = \sum_{j=1}^{(n-1)/2} \int_{x_{2j-1}}^{x_{2j+1}} |f''(x) - (n-1)^2[f(x_{2j+1}) - 2f(x_{2j}) + f(x_{2j-1})]| \, dx. \quad (7)$$

Now we bound each integral in the summation. For $j = 1, \dots, (n-1)/2$, let $\eta_j(x) = f''(x) - (n-1)^2[f(x_{2j+1}) - 2f(x_{2j}) + f(x_{2j-1})]$, and let p_j denote the probability that $\eta_j(x)$ is non-negative:

$$p_j = \frac{(n-1)}{2} \int_{x_{2j-1}}^{x_{2j+1}} \mathbb{1}_{[0, \infty)}(\eta_j(x)) \, dx,$$

and so $1 - p_j$ is the probability that $\eta_j(x)$ is negative.

It follows that

$$\begin{aligned} \int_{x_{2j-1}}^{x_{2j+1}} \max(\eta_j(x), 0) \, dx &\leq \frac{2p_j}{n-1} \sup_{x_{2j-1} \leq x \leq x_{2j+1}} \eta_j(x), \\ \int_{x_{2j-1}}^{x_{2j+1}} \max(-\eta_j(x), 0) \, dx &\leq \frac{-2(1-p_j)}{n-1} \inf_{x_{2j-1} \leq x \leq x_{2j+1}} \eta_j(x) \end{aligned}$$

These bounds allow us to derive bounds on the integrals in (7):

$$\begin{aligned} &\int_{x_{2j-1}}^{x_{2j+1}} |\eta_j(x)| \, dx \\ &= \int_{x_{2j-1}}^{x_{2j+1}} \max(\eta_j(x), 0) \, dx + \int_{x_{2j-1}}^{x_{2j+1}} \max(-\eta_j(x), 0) \, dx \\ &\leq \frac{2p_i}{n-1} \sup_{x_{2j-1} \leq x \leq x_{2j+1}} \eta_j(x) - \frac{2(1-p_i)}{n-1} \inf_{x_{2j-1} \leq x \leq x_{2j+1}} \eta_j(x) \\ &\leq \frac{2p_i(1-p_i)}{n-1} \left[\sup_{x_{2j-1} \leq x \leq x_{2j+1}} \eta_j(x) - \inf_{x_{2j-1} \leq x \leq x_{2j+1}} \eta_j(x) \right] \\ &\leq \frac{1}{2(n-1)} \left[\sup_{x_{2j-1} \leq x \leq x_{2j+1}} f''(x) - \inf_{x_{2j-1} \leq x \leq x_{2j+1}} f''(x) \right], \end{aligned}$$

since $p_i(1-p_i) \leq 1/4$.

Plugging this bound into (7) yields

$$\begin{aligned}
\|f'' - 4[f(1) - 2f(1/2) + f(0)]\|_1 - \tilde{F}_n(f) &= |f|_{\tilde{\mathcal{F}}} - \tilde{F}_n(f) \\
&\leq \|f'' - A_n(f)''\|_1 \\
&\leq \frac{1}{2(n-1)} \sum_{j=1}^{(n-1)/2} \left[\sup_{x_{2j-1} \leq x \leq x_{2j+1}} f''(x) - \inf_{x_{2j-1} \leq x \leq x_{2j+1}} f''(x) \right] \\
&\leq \frac{\text{Var}(f'')}{2(n-1)} = \frac{|f|_{\mathcal{F}}}{2(n-1)},
\end{aligned}$$

and so

$$h_+(n) := \frac{1}{2n-2}, \quad \mathfrak{C}_n = \frac{1}{1-\tau/(2n-2)} \quad \text{for } n > 1 + \tau/2.$$

Since $\tilde{F}_3(f) = 0$ by definition, the above inequality for $|f|_{\tilde{\mathcal{F}}} - \tilde{F}_3(f)$ implies that

$$4\|f' - f(1) + f(0)\|_1 = 4|f|_{\tilde{\mathcal{F}}} \leq |f|_{\mathcal{F}} = \text{Var}(f'), \quad \tau_{\min} = 4.???$$

The error of the Simpson's rule in terms of the variation of the first derivative of the integrand is:

$$\begin{aligned}
\left| \int_0^1 f(x) dx - P_n(f) \right| &\leq h(n) \text{Var}(f''') \\
h(n) &:= \frac{1}{72(n-1)^4}, \quad h^{-1}(\varepsilon) = \left\lceil \left(\frac{1}{72\varepsilon} \right)^{1/4} \right\rceil + 1.
\end{aligned}$$

Given the above definitions of $h, \mathfrak{C}_n, \mathfrak{c}_n$, and $\tilde{\mathfrak{c}}_n$, it is now possible to also specify

$$h_1(n) = h_2(n) = \mathfrak{C}_n h(n) = \frac{1}{72(n-1)^3(n-1-\tau)}, \quad (8a)$$

$$h_1^{-1}(\varepsilon) = h_2^{-1}(\varepsilon) = 1 + \left\lceil \sqrt{\frac{\tau}{8\varepsilon} + \frac{\tau^2}{16}} + \frac{\tau}{4} \right\rceil \leq 2 + \frac{\tau}{2} + \sqrt{\frac{\tau}{8\varepsilon}}.???. \quad (8b)$$

Moreover, the left side of the stopping criterion inequality in the multi-stage algorithm, becomes

$$\tau h(n_i) \mathfrak{C}_{n_i} \tilde{F}_{n_i}(f) = \frac{\tau^2 \tilde{F}_{n_i}(f)}{36(n_i-1)^3(2n_i-2-\tau)}. \quad (8c)$$

With these preliminaries, Algorithm ?? and Theorem ?? may be applied directly to yield the following adaptive integration algorithm and its guarantee.

Algorithm 1 (Adaptive Univariate Integration). Let the sequence of algorithms $\{P_n\}_{n \in \mathcal{I}}$, $\{\tilde{F}_n\}_{n \in \mathcal{I}}$, and $\{F_n\}_{n \in \mathcal{I}}$ be as described above. Let $\tau \geq 4$ be the cone constant. Set $i = 1$. Let $n_1 = 2\lceil \tau/2 \rceil + 1$. For any error tolerance ε and input function f , do the following:

Stage 1. Estimate $\|f'' - 4[f(1) - 2f(1/2) + f(0)]\|_1$ **and bound** $\text{Var}(f''')$. Compute $\tilde{F}_{n_i}(f)$ in (5) and $F_{n_i}(f)$ in (6).

Stage 2. Check the necessary condition for $f \in \mathcal{C}_\tau$. Compute

$$\tau_{\min, n_i} = \frac{F_{n_i}(f)}{\tilde{F}_{n_i}(f) + F_{n_i}(f)/(2n_i - 2)}.$$

If $\tau \geq \tau_{\min, n_i}$, then go to stage 3. Otherwise, set $\tau = 2\tau_{\min, n_i}$. If $n_i \geq (\tau + 1)/2$, then go to stage 3. Otherwise, choose

$$n_{i+1} = 1 + (n_i - 1) \left\lceil \frac{\tau + 1}{n_i - 1} \right\rceil.$$

Go to Stage 1.

Stage 3. Check for convergence. Check whether n_i is large enough to satisfy the error tolerance, i.e.

$$\tilde{F}_{n_i}(f) \leq \frac{36\varepsilon(n_i - 1)^3(2n_i - 2 - \tau)}{\tau}.$$

If this is true, then return $T_{n_i}(f)$ and terminate the algorithm. If this is not true, choose

$$n_{i+1} = 1 + (n_i - 1) \max \left\{ 2, \left\lceil \frac{1}{(n_i - 1)} \sqrt{\frac{\tau \tilde{F}_{n_i}(f)}{8\varepsilon}} \right\rceil \right\} . ???$$

Go to Stage 1.