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Local adaption for approximation and minimization of univariate functions[☆]

Sou-Cheng T. Choi [a], Yuhan Ding [a], Fred J. Hickernell [a,*], Xin Tong [b]

[a] *Department of Applied Mathematics, Illinois Institute of Technology, RE 208, 10 West 32nd Street, Chicago, IL, 60616, USA*

[b] *Department of Mathematics, Statistics, and Computer Science, University of Illinois at Chicago, Room 322 SEO, 851 S. Morgan Street, Chicago, IL, 60607, USA*

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ABSTRACT

Most commonly used *adaptive* algorithms for univariate real-valued function approximation and global minimization lack theoretical guarantees. Our new locally adaptive algorithms are guaranteed to provide answers that satisfy a user-specified absolute error tolerance for a cone, $\mathcal{C}$, of non-spiky input functions in the Sobolev space $W^{2,\infty}[a, b]$. Our algorithms automatically determine where to sample the function—sampling more densely where the second derivative is larger. The computational cost of our algorithm for approximating a univariate function f on a bounded interval with L^∞-error no greater than ε is $\mathcal{O}\left(\sqrt{\|f''\|_{\frac{1}{2}}/\varepsilon}\right)$ as $\varepsilon \to 0$. This is the same order as that of the best function approximation algorithm for functions in $\mathcal{C}$. The computational cost of our global minimization algorithm is of the same order and the cost can be substantially less if f significantly exceeds its minimum over much of the domain. Our Guaranteed Automatic Integration Library (GAIL) contains these new algorithms. We provide numerical experiments to illustrate their superior performance.

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* Corresponding author.
E-mail address: hickernell@iit.edu (F.J. Hickernell).

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1. Introduction

Our goal is to reliably solve univariate function approximation and global minimization problems by adaptive algorithms. We prescribe a suitable set, $\mathcal{C}$, of continuously differentiable, real-valued functions defined on a finite interval $[a, b]$. Then, we construct algorithms $A : (\mathcal{C}, (0, \infty)) \to L^\infty[a, b]$ and $M : (\mathcal{C}, (0, \infty)) \to \mathbb{R}$ such that for any $f \in \mathcal{C}$ and any error tolerance $\varepsilon > 0$,

$$\|f - A(f, \varepsilon)\| \le \varepsilon, \tag{APP}$$

$$0 \le M(f, \varepsilon) - \min_{a \le x \le b} f(x) \le \varepsilon. \tag{MIN}$$

Here, $\|\cdot\|$ denotes the L^∞-norm on $[a, b]$, i.e., $\|f\| = \sup_{x\in[a,b]} |f(x)|$. Algorithms A and M depend only on function values.

Our algorithms proceed iteratively until their data-dependent stopping criteria are satisfied. The input functions are sampled nonuniformly over $[a, b]$, with the sampling density determined by the function data. We call our algorithms *locally adaptive*, to distinguish them from globally adaptive algorithms that have a fixed sampling pattern and only the sample size determined adaptively.

1.1. Key ideas in our algorithms

Our Algorithms A and M are based on a *linear spline*, $S(f, x_{0:n})$ defined on $[a, b]$. Let $0 : n$ be shorthand for $\{0, \dots, n\}$, and let $x_{0:n}$ be any ordered sequence of $n + 1$ points that includes the endpoints of the interval, i.e., $a =: x_0 < x_1 < \cdots < x_{n-1} < x_n := b$. We call such a sequence a *partition*. Then given any $x_{0:n}$ and any $i \in 1 : n$, the linear spline is defined for $x \in [x_{i-1}, x_i]$ by

$$S(f, x_{0:n})(x) := \frac{x - x_i}{x_{i-1} - x_i} f(x_{i-1}) + \frac{x - x_{i-1}}{x_i - x_{i-1}} f(x_i). \tag{1}$$

The error of the linear spline is bounded in terms of the second derivative of the input function as follows [2, Theorem 3.3]:

$$\|f - S(f, x_{0:n})\|_{[x_{i-1},x_i]} \le \frac{(x_i - x_{i-1})^2 \left\|f''\right\|_{[x_{i-1},x_i]}}{8}, \quad i \in 1 : n, \tag{2}$$

where $\|f\|_{[\alpha,\beta]}$ denotes the L^∞-norm of f restricted to the interval $[\alpha, \beta] \subseteq [a, b]$. This error bound leads us to focus on input functions in the Sobolev space $W^{2,\infty} := W^{2,\infty}[a, b] := \{f \in C^1[a, b] : \left\|f''\right\| < \infty\}$.

Algorithms A and M require upper bounds on $\left\|f''\right\|_{[x_{i-1},x_i]}$, $i \in 1 : n$, to make use of (2). A nonadaptive algorithm might assume that $\left\|f''\right\| \le \sigma$, for some known σ, and proceed to choose $n = \left\lceil (b - a)\sqrt{\sigma/(8\varepsilon)} \right\rceil$, $x_i = a + i(b - a)/n$, $i \in 0 : n$. Providing an upper bound on $\left\|f''\right\|$ is often impractical, and so we propose adaptive algorithms that do not require such information.

However, one must have some a priori information about $f \in W^{2,\infty}$ to construct successful algorithms for (APP) or (MIN). Suppose that Algorithm A satisfies (APP) for the zero function $f = 0$, and $A(0, \varepsilon)$ uses the data sites $x_{0:n} \subset [a, b]$. Then one can construct a *nonzero* function $g \in W^{2,\infty}$ satisfying $g(x_i) = 0$, $i \in 0 : n$ but with $\|g - A(g, \varepsilon)\| = \|g - A(0, \varepsilon)\| > \varepsilon$.

Our set $\mathcal{C} \subset W^{2,\infty}$ for which A and M succeed includes only those functions whose second derivatives do not change dramatically over a short distance. The precise definition of $\mathcal{C}$ is given in Section 2. This allows us to use second-order divided differences to construct rigorous upper bounds on the linear spline error in (2). These data-driven error bounds inform the stopping criteria for Algorithm A in Section 3.1 and Algorithm M in Section 4.1.

The computational cost of Algorithm A is analyzed in Section 3.2 and is shown to be $\mathcal{O}\left(\sqrt{\|f''\|_{\frac{1}{2}}/\varepsilon}\right)$ as $\varepsilon \to 0$. Here, $\|\cdot\|_{\frac{1}{2}}$ denotes the $L^{\frac{1}{2}}$-quasi-norm, a special case of the L^p-quasi-norm, $\|f\|_p := \left(\int_a^b |f|^p \, dx\right)^{1/p}$, $0 < p < 1$. Since $\left\|f''\right\|_{\frac{1}{2}}$ can be much smaller than $\left\|f''\right\|$, locally adaptive

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