Approximation of the inverse of a function near an extremum

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Introduction

Consider a twice differentiable function $f : \mathbb{R} \to \mathbb{R}$ and an interval of interest $X = [\underline{x}, \overline{x}]$ containing a single stationary point x^* of f, i.e., $f'(x) \neq 0$ for all $x \in X \setminus \{x^*\}$. This situation typically occurs in branch-and-bound algorithms when a (local) optimizer is isolated. In this situation, constraint contractors based on the inverse of f become inefficient because of the infinite derivative of f^{-1} at x^*.

Let $Y = f(X)$ be the interval image of X by f (necessarily a bounded subset of $\mathbb{R}$) and $y^* = f(x^*)$. Since it has no other stationary points, f is necessarily strictly monotonous on the left $X_l = [\underline{x}, x^*]$ and right $X_r = [x^*, \overline{x}]$ parts of X. It follows f^{-1} is also strictly monotonous on $Y_l = f(X_l) = [\min(f(\underline{x}), y^*), \max(f(\underline{x}), y^*)]$ and on $Y_r = f(X_r) = [\min(f(\overline{x}), y^*), \max(f(\overline{x}), y^*)]$. Without loss of generality, we will consider only the approximation of f^{-1} on Y_r in the case where f is strictly increasing on X_r and $x^* = y^* = 0$. All other cases can be addressed similarly.

Our motivation comes from the Gibbs entropy function, used in thermodynamics, defined as $S(x) = x \log x + (1 - x) \log(1 - x)$. Since S is not differentiable at $x = 0$ and $x = 1$, we consider $X = [0.05, 0.95]$.

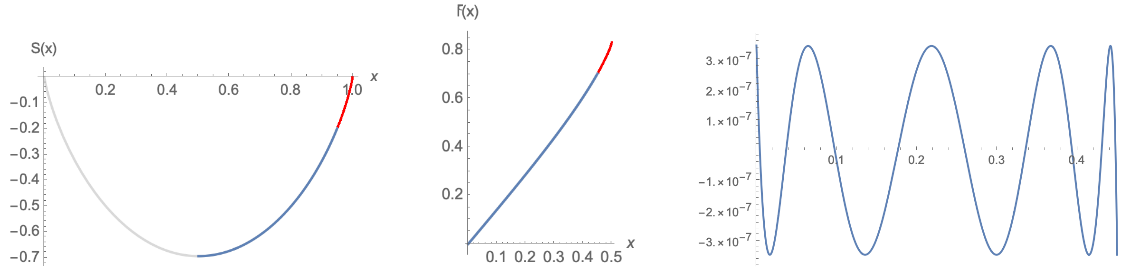

Figure 1: Left, Gibbs entropy function S. Middle, its reformulation F. Right, approximation error of a near optimal degree 8 polynomal approximation of F^{-1}.

Furthermore, in order to make it more amenable to polynomial approximation, we consider the reformulation $F(x) = \sqrt{S(x+0.5)+\ln 2}$ on $X = [0, 0.45]$, i.e., the right part of a quadratic scaling of S with minimum transposed at $x^* = y^* = 0$. Figure 1 depicts S and F.

We propose in this presentation a method to compute an optimal polynomial approximation p of the inverse of f on X.

Inverse approximation formulations

Univariate optimal-error polynomial approximation, *a.k.a.* Chebyshev approximation [2], consists in finding the coefficients $a \in \mathbb{R}^{n+1}$ of a polynomial p of degree n that minimize the extrema of the approximation error function $e(a,x) = f(x) - p_a(x)$. It is usually formulated as a minimax optimization problem, which, applied to inverse function approximation, becomes

$$\min_{a\in\mathbb{R}^{n+1}} \max_{y\in[0,\overline{y}]} |f^{-1}(y) - p_a(y)|, \tag{1}$$

which can be reformulated as

$$\min_{a\in\mathbb{R}^{n+1}} \max_{x\in[0,\overline{x}]} |x - p_a(f(x))|. \tag{2}$$

The latter formulation has two advantages: it does not require the expression of f^{-1} in order to compute a; and it has the general form of a linear semi-infinite program (LSIP) and can thus be treated using regular exchange algorithms, e.g., the second Remez algorithm [4], already implemented in tools like Sollya [3]. This tool uses interval computations with arbitrary precision and can find very precisely the optimal polynomial approximation p_a^*, i.e., the one that exhibits equioscillation of the error function.

For example, Sollya computes the following degree 8 polynomial approximation of F^{-1} in 0.85 second on a standard laptop:
$p(x) = -3.4598005 \times 10^{-7} + 0.7071781x - 0.0024082x^2 - 0.0867757x^3$
$-0.1976639x^4 + 0.6613514x^5 - 1.3349492x^6 + 1.3591456x^7$
$- 0.5938170x^8$.
Its approximation error function is depicted in Figure 1(right): it exhibits a near perfect equioscillation with 10 extremum (including the two bounds, $y = 0$ and $y = 0.45$).

Bounding the approximation error

Due to the inifinite derivative of the inverse function at y^*, tools like Sollya can only provide an approximate error bound on the computed polynomial approximation. However, it is mandatory to obtain a guaranteed upperbound of the maximum error in order to substitute rigorously an inverse function for its polynomial approximation within a constraint contractor.

To this end, we use a global interval solving method, like the ones implemented in Ibex [1], to solve the following problem:

$$\max_{x \in [0,\overline{x}]} |x - p_a^*(f(x))|. \tag{3}$$

Applied to the Gibbs entropy function, Ibex validates a guaranteed upperbound 3.5897×10^{-7} on the considered domain $[0, 0.45]$ in 3.45 seconds on a standard laptop.

References

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