Efficient Approximation of Implicitly Defined Functions: General Theorems and Classical Benchmark Studies

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Abstract

The traditional techniques of approximation theory in the form of kernel interpolation and cubic spline approximation are used to obtain representations and estimates for functions implicitly defined as solutions of two-point boundary-value problems. We place this benchmark analysis in the following more general context: the approximation of operator fixed points, not known in advance, through a balanced combination of discretization and iteration. We have chosen to make use of the pendulum and elastica equations, linked by the Kirchhoff analogy, to illustrate these ideas. In the study of these important classical models, it is approximation theory, not numerical analysis, which is the required theory; a significant example from micro-biology is cited related to nucleosome repositioning. In addition, other suggested uses of approximation theory emerge. In particular, the determination of approximations via symbolic calculation programs such as Mathematica is proposed to facilitate exact error estimation. No numerical linear *inversion* is required to compute the approximations in any case. The basic premise of the paper is that approximations should be exactly computable in function form (up to round-off error), with error estimated in a smooth averaged norm. Functional analysis is employed as an effective organizing principle to achieve this 'a priori' estimation.

Key words: Approximation, iteration, discretization, interpolation, contraction mapping theorem, Newton-Kantorovich theorem, pendulum equation, Green's function, elastica.
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1 Introduction

Fixed point theorems and theorems which predict zeros of nonlinear mappings occupy a central position in mathematical analysis and its applications. Two constructive theorems, which also serve as tools to prove existence, are:

1. The Banach contraction mapping theorem [4];

2. The Newton-Kantorovich theorem [8].

The Schauder fixed point theorem, which is the natural generalization to infinite dimensional spaces of the Brouwer theorem, is non-constructive, and would appear to have no direct use in computation. However, it can be effectively used in conjunction with the convergence of numerical fixed points; a useful such theory is due to Krasnosel'skii et al [12]. One can think of a numerical fixed point as the solution of a discretization scheme.

Various combinations of these theorems have been employed to analyze complex models. This article will illustrate the interplay of the ideas above with iteration and discretization. It may be viewed as a sequel to [10].

In order to present the ideas effectively, we employ a classical bench-mark example, the two-point boundary-value problem defining a quarter period of the undamped oscillating pendulum. This may also be interpreted, via Kirchhoff's kinetic analog (see [11, 16]), as an equilibrium position for the elastica. The pendulum equation is nonlinear, but possesses a structure sufficiently transparent for illustration. The original results of the paper include the central Theorem 4 providing an 'a priori' estimate of the accuracy of an explicit approximation to a fixed point known only implicitly. We also obtain approximation representations and estimates for the pendulum equation and the elastica never obtained previously, in terms of cubic spline approximation, and a variational characterization of the elastica required by the kinetic analog. The derived formulas permit symbolic calculation and completely bypass numerical linear algebra, so that no inversion is required for the approximations. Moreover, the goal goes well beyond the numerical solution of two-point boundary-value problems. There exist reliable software packages for this, such as AUTO and CONTENT. What we require is an approximation theory, including analytical approximations. For example, in the formation of loops in the repositioning of nucleosomes along DNA (see [13]), the loops are approximated via the circle-line approximation, depending locally on curvature. The analysis of this paper may be seen to give rise to a more sophisticated analytical approximation, and may find some systematic use in this, and similar applications.

2 The Pendulum Equation

In the first two sections, we discuss the applications: the oscillating pendulum and the elastica.

2.1 The Oscillating Pendulum

Consider the boundary-value problem for the well-known (undamped) pendulum equation [3, pp. 217-218],

$$-\ell\ddot{\theta}(t) = \cos\theta(t),\ 0 \le t \le \bar{t},\ \theta(0) = 0,\ \theta(\bar{t}) = -\pi, \tag{2.1}$$

where ℓ denotes the length of the pendulum, subjected to unit gravitational force g downward. The pendulum swings in a fixed plane along a circle with displacement $\ell\theta$, starting from horizontal position $\theta = 0$ with velocity $\dot{\theta} = 0$ at time $t = 0$, and reaching velocity $\dot{\theta} = 0$ again at $t = \bar{t}$ when $\theta = -\pi$. This swing constitutes a half-period. It is useful to consider the canonical case $\ell = 2$ and to track the pendulum only during the first half of its swing. Thus we get the two-point boundary-value problem,

$$-\ddot{\theta} = \frac{1}{2}\cos\theta,\ \theta(0) = 0,\ \theta(L) = -\pi/2,\ \ (L = \bar{t}/2). \tag{2.2}$$

Because we choose standard coordinates, with θ the angle made by the pendulum with respect to the positive x-axis, θ will assume values between 0 and $-\pi/2$. Equation (2.2) is also characterized variationally as the Euler-Lagrange equation satisfied by critical points of the Lagrangian. For the interested reader, a formal derivation of Hamilton's principle, and of the Euler-Lagrange equations is given in [17], where a derivation of the system for the double pendulum is carried out (see section 5.5 of [17]). There is also a discussion of the single pendulum in [22, Ex. 2, p. 255]. We shall see presently that the Banach contraction mapping theorem applies to the boundary-value problem.

2.2 Elastica Configurations

Elastica are critical curves of the strain energy, $\int_0^1 \kappa^2 \, ds$, where κ is the curvature. Suitable constraints on the curves produce a boundary-value problem in the form of the pendulum equation (see [7] for an early study). The relationship between (2.2) and elastica configurations is clarified with the help of Jacobi elliptic functions (see [14] for a discussion of these functions). Moreover, *Mathematica* provides built-in Jacobi elliptic functions and elliptic integrals; see [15] for its applications to elastic curves. The unique solution of (2.2) occurs (using the convention of *Mathematica* with $m = 1/2$) when $\sqrt{m}L$ is the quarter period of the Jacobi elliptic function $\mathrm{sn}(\cdot\,; m)$. In this case, the solution is given explicitly by

$$\theta(t) = -\pi/2 - 2 \arcsin[\sqrt{m}\, \mathrm{sn}(\sqrt{m}(t - L); m)], \; 0 \leq t \leq L.$$

Mathematica gives the approximate value $L = 2.62206$ when $L = K_m/\sqrt{m}$ and K_m is the complete elliptic integral of the first kind. With this value of L, the three conditions, $\theta(0) = 0, \dot{\theta}(0) = 0, \theta(L) = -\pi/2$ are satisfied.

It is of interest whether this equation and boundary conditions, with their unique solution, can be replicated by an elastica, especially since these curves are significant tools in approximation theory.

The elastica is to have representation

$$x(s) = h\cos\theta(s),\ 0 \le s \le 1, y(s) = h\sin\theta(s),\ 0 \le s \le 1,$$

for h to be determined. We give the details of the derivation in the appendix, but indicate the essential facts here.

Change parameter from time t to arclength s according to $t = \sqrt{2}\,K_m s$ so that

$$\tilde{\theta}(s) = -\tfrac{\pi}{2} - 2\arcsin[\sqrt{m}\ \mathrm{sn}(K_m(s-1); m)],$$

and $\tilde{\theta}''(s) = -K_m^2\cos\tilde{\theta}(s)$. This kinetic transformation gives an effective length of unity for the elastica, which has its initial position at the origin, and extends downward. It is shown in the appendix how this curve arises from the critical point equations, augmented by a constraint on the y-coordinate h of the terminal point of the elastica, to guarantee the boundary conditions. This value is $h \approx -0.456947$. For this particular value, there is an elastic curve that starts horizontally, and then bends downward until it reaches the 'height' h, at which point its tangent is vertical. Moreover, the curvature at the initial point vanishes, and the tangent angle $\tilde{\theta}(s)$ agrees with the pendulum's deflection angle $\theta(t)$ at time $t = \sqrt{2}\,K_m s$ when the length of the pendulum satisfies $l = 2$.

2.3 Green's Function Formulation

We can rewrite the boundary-value problem (2.2) by use of the Green's function [18, Sec. 8.1] $G(t,s)$:

$$\theta(t) = \int_0^L G(t,s)\left[\frac{1}{2}\cos\theta(s)\right]\ ds\ -\frac{\pi t}{2L},\ 0 \le t \le L. \tag{2.3}$$

G is a continuous symmetric kernel on the square $S = [0,L] \times [0,L]$, satisfying $G(t,s) = \frac{1}{L}s(L-t),\ 0 \le s \le t$, with symmetric continuation for $t \le s \le L$. The Green's function is the kernel of the operator $\mathcal{G}$, which is a continuous linear operator on $L_2(0,L)$, with norm $\|\mathcal{G}\|$ bounded by the expression

$$\left\{ \int_S |G(t,s)|^2 \, dtds \right\}^{1/2} = .724708.$$

By $L_2(0, L)$ we mean the linear space of real Lebesgue measurable functions on $(0, L)$, which are square integrable, with inner product:

$$(f, g)_2 = \int_0^L f(t)g(t) \, dt.$$

We refer to the classic reference [1] for basic facts concerning L_2 and Hilbert space linear operators. The operator $\mathcal{G}$ is actually an operator of Hilbert-Schmidt type. It serves as the inverse of the closed linear operator $-\frac{d^2}{dt^2}$, with domain consisting of functions u, with two L_2 derivatives, such that $u(0) = u(L) = 0$.

2.4 Fixed Point Framework: Contraction Mapping

If we write $T\theta$ for the r.h.s. of (2.3), so that it may be represented as

$$\theta(t) = (T\theta)(t) = \int_0^L G(t,s) \left[\frac{1}{2} \cos \circ \theta(s) \right] \, ds \; - \frac{\pi t}{2L}, \tag{2.4}$$

then we have identified the solution as a fixed point of the nonlinear mapping T. The choice of normed space on which T is defined is flexible; $L_2(0, L)$ would work. However, because of later comparisons with the discretization T_N of T, it is more appropriate to employ a smooth Hilbert space, which we describe now. Define the Sobolev space

$$H^2(0, L) = \{f : f, f', f'' \in L_2(0, L)\},$$

with inner product

$$(f, g)_{H^2} = (f'', g'')_2 + f(0)g(0) + f(L)g(L).$$

By the preceding theory, we can recover f from f'' via

$$f(t) = \mathcal{G}f''(t) + f(0) + (f(L) - f(0))(t/L). \tag{2.5}$$

This technique allows us to use the completeness of L_2 to infer the completeness of H^2. We introduce some additional notation. We define the closed subspace,

$$H_0^2(0,L) = \{f \in H^2(0,L) : f(0) = 0, f(L) = 0\}. \tag{2.6}$$

This deviates from standard notation: no endpoint conditions are assumed for the derivatives. If Lin denotes the two-dimensional space of linear functions $p(s) = A + Bs$ on $[0, L]$, we consider the orthogonal sum within H^2, given by

$$\mathcal{H} = H_0^2 \oplus \mathrm{Lin} = H^2(0,L).$$

Throughout this paper, we shall consider T as acting on the set,

$$\mathcal{U} = \{f \in \mathcal{H} : f(0) = 0, f(L) = -\pi/2\}, \tag{2.7}$$

which describes the boundary conditions of (2.2). This is the natural metric space containing the domain and range of T. Thus, $T : \mathcal{U} \mapsto \mathcal{U}$,

$$Tf(t) = \int_0^L G(t,s) \left[\frac{1}{2}\cos\circ f(s)\right] ds \; - \frac{\pi t}{2L}, \; 0 \le t \le L.$$

We now proceed to estimate the contraction constant of T.

Lemma 1. *The domain $\mathcal{U}$ of T is a closed affine subset of $\mathcal{H}$. The contraction constant of T is $C = .362354$. In particular, there is a unique fixed point θ of T in $\mathcal{U}$. This function is the unique solution of (2.2).*

Proof. The affine property of $\mathcal{U}$ is immediate from the representation,

$$\mathcal{U} = \theta_0 + H_0^2(0,L),$$

where $\theta_0(s) = -\pi s/(2L)$. The property that $\mathcal{U}$ is closed follows from (2.5). To estimate the contraction constant, we note that $\phi \mapsto \cos\phi$ is non-expansive on $L_2(0,L)$, so that the definition gives

$$\|T\phi - T\psi\|_{H^2} \le \frac{1}{2}\|\phi - \psi\|_2 \le C\|\phi - \psi\|_{H^2}, \tag{2.8}$$

if $\phi, \psi \in \mathcal{U}$. Here, we have used the estimate,

$$\frac{1}{2}\|\phi - \psi\|_2 \leq \frac{1}{2}\left\{\int_S |G(t,s)|^2 \, dtds\right\}^{1/2} \|\phi - \psi\|_{H^2} = C\|\phi - \psi\|_{H^2}, \; C = .362354. \quad (2.9)$$

Since $\mathcal{U}$ is a complete metric space, and $C < 1$, we have the hypotheses of the contraction mapping theorem [4], which yields a unique fixed point. □

2.5 Successive Approximation

If we define θ_0 as above, and $\theta_n = T\theta_{n-1}, \; n = 1, 2, \ldots,$ then $\theta_n \in \mathcal{U}, n \geq 0$. According to the estimates of the contraction mapping principle, the successive approximations θ_n are convergent to the unique fixed point $\theta \in \mathcal{U}$ and the estimate,

$$\|\theta_n - \theta\|_{H^2} \leq \frac{C^n}{1 - C}\|\theta_1 - \theta_0\|_{H^2}, \;\; n = 1, \ldots, \quad (2.10)$$

is valid. We readily estimate:

$$\|\theta_1 - \theta_0\|_{H^2} = \frac{1}{2}\|\cos \circ \theta_0\|_2,$$

so that we obtain

$$\|\theta_n - \theta\|_{H^2} \leq \frac{1}{2}\frac{C^n}{1 - C}\|\cos \circ \theta_0\|_2, \text{ where}$$

$$\|\cos \circ \theta_0\|_2 = 1.145. \quad (2.11)$$

When $n = 1$, (2.11) gives an upper estimate of .325334 for $\|\theta_1 - \theta\|_{H^2}$. If we wish accuracy to within a norm error of .1, we require iteration through θ_3: In this case, we have the estimate,

$$\|\theta_3 - \theta\|_{H^2} \leq .0427165.$$

This is a viable bound only if θ_3 is analytically representable. However, this is problematical, since the computation involves both the composition in defining the integrand, as well the integral,

$$\theta_n(t) = \frac{1}{2}\int_0^L G(t,s) \cos \circ \theta_{n-1}(s) \, ds - \frac{\pi t}{2L}.$$

2.6 Approximation of the Recursion

Although θ_1 is analytically computable, this is not the case for iterates beyond $n = 1$. One might consider power series expansions of $\cos\theta$ in order to compute this integral, but this complicates error estimation as the iteration proceeds; in addition, since θ_{n-1} is a function of s, a uniform polynomial approximation of $\cos(\cdot)$ of degree m expands to a polynomial of degree $O(m^{n-1})$ by the completion of the n-th iteration. One first encounters this in computing θ_2. Instead, compute θ_2 as follows. Given the equally spaced points (uniform grids are not essential, simply convenient): $t_i = ih$ of $[0, L]$, $i = 0, \ldots, N + 1$, introduce the piecewise linear interpolant γ_1, linear on $[t_{i-1}, t_i]$, and satisfying $\gamma_1(t_i) = \cos \circ\, \theta_1(t_i), i = 0, \ldots, N + 1$. Define an approximation to θ by

$$\frac{1}{2}\int_0^L G(t,s)\gamma_1(s)\,ds - \frac{\pi t}{2L},$$

and thereby obtain a C^2 cubic spline, with 'knots' at the nodal points $t_i, i = 1, \ldots, N$, which can be exactly expressed by an analytical formula, and will be adopted as the basis for our discretization of T. It is directly computable by *Mathematica*, for example. We refer to [2] for an introduction to this important subject, and [20] for additional exposition. We now systematically develop the discretization.

2.7 The Discretization of T

We first introduce some notation. The affine space $\mathcal{U}$ is contained in $\mathcal{H}$. Further, if the spline space is described as

$$\mathcal{S} = \{q : q \in C^2[0,L] :\ q_{|[t_{i-1},t_i]} \text{ is a cubic polynomial}, i = 1, \ldots, N{+}1,\ q(0) = q(L) = 0\}, \tag{2.12}$$

we define E_N to be the orthogonal sum of $\mathcal{S}$ and Lin:

$$E_N = \mathcal{S} \oplus \mathrm{Lin} \subset \mathcal{H}.$$

Analogous to the contraction mapping T, one has the contraction mapping T_N, defined on the affine space $\mathcal{U}_N = \mathcal{U} \cap E_N$:

$$T_N \phi(t) = \frac{1}{2} \int_0^L G(t,s) I_N \cos \circ \phi(s) \, ds - \frac{\pi t}{2L}. \tag{2.13}$$

Here I_N denotes the interpolation operator acting on $f = \cos \circ \, \phi$. Thus, $I_N f$ is linear on $[t_{i-1}, t_i]$, and satisfies $I_N f(t_i) = f(t_i), i = 0, \dots, N+1$. The contraction constant is described in Lemma 6 to follow. Let us return to the earlier question of computing an approximation of θ with error not exceeding .1 in the H^2 metric. By employing the computable operator T_N, one is really approximating the fixed point of T_N on E_N. Note that the 'hidden' assumption is that exact evaluation of the cosine is possible at $\phi(t_i)$ in (2.13). This simply means that we have exactness, up to the precision of the computer arithmetic. This (roundoff) error is not considered in this article. One can repeat this process for appropriate choice of $h = L/(N+1)$. At the third stage, we compute an approximation ψ_3 to θ_3, but the 'discretization' error has entered, and we are uncertain whether our calculated approximation lies within a tolerance of .1. In this case, we know the exact solution, and can check, but this is not possible in more complicated cases. We are led to inquire whether there are any general principles for doing this. We shall investigate this now in a general framework.

3 Nonlinear Operator Approximation

Given a Banach space X and a subset U of X, suppose T is a mapping from U into X with a fixed point:

$$Tx_0 = x_0.$$

The reader may conveniently make the identification $x_0 = \theta$. If $\{X_N\}$ denotes a sequence of subspaces of X of finite dimension $r(N) \geq N$, suppose that $U_N = U \cap X_N$ and that

$T_N : U_N \mapsto X_N$, has a fixed point:

$$T_N x_N = x_N.$$

Suppose we have an algorithm, such as can be obtained from (2.13) with $\phi \mapsto \psi_{n-1}$, which permits the calculation of approximations $\tilde{x}_N$ of x_N. The ultimate question is the accuracy of approximation of x_0 itself. We proceed to answer this question.

3.1 Zeros of Smooth Mappings

We first record a general proposition on the zeros of C^1 mappings, followed by a corollary adapted to the present situation. The proposition is a restatement, with slight modifications, of [12, Lemma 19.1]. The principal use of C^1 differentiability is the operator mean value theorem [12, p. 12]. Recall that C^1-Fréchet differentiability is equivalent to C^1-Gateaux differentiability.

Proposition 2. *Let X be a Banach space and let A be an operator, with domain an open set Ω in X and range in X, which possesses a C^1-Gateaux derivative with respect to directions $u \in X$, denoted*

$$A'(x)[u] = \lim_{\epsilon \to 0} \left(\frac{A(x + \epsilon u) - A(x)}{\epsilon} \right), \; x \in \Omega, \; u \in X.$$

In particular, $A'(x)$ is a bounded linear operator on X for each $x \in \Omega$ and A' is continuous in the uniform operator topology on X and satisfies the mean value theorem. Suppose, for some $x_* \in \Omega$, $[A'(x_*)]^{-1}$ exists as a bounded linear operator on X, and that the following conditions hold:

$$\sup_{\|x - x_*\| \leq \delta_0} \|[A'(x_*)]^{-1}[A'(x) - A'(x_*)]\| \leq q, \tag{3.1}$$

$$\alpha := \|[A'(x_*)]^{-1} A(x_*)\| \leq \delta_0 (1 - q), \tag{3.2}$$

for some δ_0 and $0 < q < 1$. Then the equation $Ax = 0$ has a unique solution x_0 in the closed ball of radius δ_0: $\|x_0 - x_*\| \leq \delta_0$.

Proof. The proof, as described in [12], relies on the construction of the operator,

$$Bx = x_* - [A'(x_*)]^{-1}\{Ax_* + [Ax - Ax_* - A'(x_*)(x - x_*)]\}.$$

The hypotheses imply that B maps the closed ball $\|x - x_*\| \leq \delta_0$ into itself, with contraction constant $q < 1$. The unique fixed point is the unique zero of A in the ball. The principal tool is the mean value theorem. Details may be found in [12]. □

There is an important corollary, pertinent to the application we are considering.

Corollary 3. *Suppose the mapping A of the proposition has the property that its restriction A_0 to $\Omega_0 = \Omega \cap \{x_* + X_0\}$ has range in X_0, where X_0 is a closed subspace of X. Define $B_{\delta_0} := \{y \in X_0 : \|y\| \leq \delta_0\}$, and suppose that the mapping $S : B_{\delta_0} \mapsto X_0$,*

$$Sy = A_0(x_* + y),\ y \in B_{\delta_0},$$

is continuously differentiable, so that $S'(y)$ is a bounded linear operator from X_0 to X_0 for each $y \in B_{\delta_0}$. Suppose the derivative maps satisfy the inequalities

$$\sup_{y \in B_{\delta_0}} \|[S'(0)]^{-1}[S'(y) - S'(0)]\| \leq q, \tag{3.3}$$

$$\alpha := \|[S'(0)]^{-1}S(0)\| \leq \delta_0(1 - q), \tag{3.4}$$

for some $0 < q < 1$. Then a unique solution x exists in $x_* + B_{\delta_0}$, satisfying $A_0x = 0$.

Proof. The proposition is applied to the mapping S, yielding a unique $y \in B_{\delta_0}$ such that $Sy = 0$. We note that $x = x_* + y$ satisfies $A_0x = 0$. □

The effectiveness of the proposition lies in the precision of its formulation. The corollary is particularly formulated for the application of this paper. We now illustrate its use in obtaining error estimates.

3.2 An Error Estimate for the Fixed Point

We shall identify x_* with an approximate fixed point $\tilde{x}_N$ of T_N. We can prove the following.

Theorem 4. *Let X be a Banach space and X_0 a closed subspace of X, let $\tilde{x}_N$ be given (as an approximate fixed point of T_N) and define the affine space $\mathcal{U} = \tilde{x}_N + X_0$. Suppose $T : \mathcal{U} \mapsto \mathcal{U}$ is differentiable in the sense*

$$T'(x)[y] = \lim_{\epsilon \to 0} \left(\frac{T(x+\epsilon y) - T(x)}{\epsilon} \right), \; x \in \mathcal{U}, \; y \in X_0,$$

exists as a bounded linear operator on X_0 for each $x \in \mathcal{U}$. Suppose that T' is Lipschitz continuous on the intersection of $\mathcal{U}$ with the closed ball $B_R(\tilde{x}_N)$ in X of radius R, in the uniform operator topology, with Lipschitz constant λ. Suppose that $[I - T'(\tilde{x}_N)]$ is invertible, and define the numbers

$$\alpha = \|[I - T'(\tilde{x}_N)]^{-1}(\tilde{x}_N - T\tilde{x}_N)\|, \; \kappa = \|[I - T'(\tilde{x}_N)]^{-1}\|.$$

If these are sufficiently small so that

$$\epsilon = 4\alpha\kappa\lambda < 1, \tag{3.5}$$

define

$$q = \frac{1}{2}\left(1 - \sqrt{1-\epsilon}\right), \; \delta = \frac{q}{\lambda\kappa}.$$

We suppose, for consistency, that $\delta \leq R$. It follows that T has a unique fixed point x_0 in the ball of radius δ centered at $\tilde{x}_N$ in $\mathcal{U}$.

Proof. We shall use the corollary and the identifications $A \mapsto I - T, x_* \mapsto \tilde{x}_N, \delta_0 \mapsto \delta$. The mapping $S : X_0 \mapsto X_0$ is now defined by $Sy = (I - T)(\tilde{x}_N + y), \; y \in X_0$. The hypothesis (3.3) of the corollary follows from the hypothesis of Lipschitz continuity for T' and from the definitions of δ, λ, κ. The hypothesis (3.4) follows from the direct calculation,

$$\alpha = \frac{q(1-q)}{\lambda\kappa} = \delta(1-q).$$

Note that we have used the algebraic fact that $q(1-q) = \epsilon/4$, together with (3.5). The corollary is now applicable, and the theorem follows with the cited identifications. $\square$

The reader may be surprised that the hypotheses make no direct assumption upon T_N. However, the estimation of $\|\tilde{x}_N - T\tilde{x}_N\|$, implicit in the requirement that $\epsilon < 1$, requires this. Typically, one uses the triangle inequality:

$$\|\tilde{x}_N - T\tilde{x}_N\| \leq \|\tilde{x}_N - T_N\tilde{x}_N\| + \|T\tilde{x}_N - T_N\tilde{x}_N\|. \tag{3.6}$$

Calibration of error

The two right hand side terms in (3.6) indicate how iteration and discretization should be balanced. The first term on the r.h.s. is strictly governed by the speed of the iteration convergence for T_N. The second term depends on the discretization error. In principle, the two terms should be of comparable size.

3.3 Synopsis of the Estimation

We have defined T_N in (2.13). In order to avoid possible confusion between the iteration index, designated by n, and the discretization, described by $h = L/(N+1)$, we shall reserve the use of these symbols to this interpretation. In the following sections, we will use Theorem 4 to estimate the error in selecting an approximation defined by T_N, for N fixed. We are retaining the notation, $\psi_n = T_N\psi_{n-1}$. This involves the following steps.

1. Estimate κ by a truncated Neumann series.

2. Estimate the Lipschitz constant λ for T'.

3. Estimate α by using the estimate for κ and estimating $\|\psi_n - T\psi_n\|_{H^2}$.

4. Test for $\epsilon < 1$, and, if valid, calculate q and δ.

5. Test for $\delta < tol$, the prescribed tolerance or error bound.

There are two principal iterative strategies studied in this paper: Picard iteration, based upon the contraction mapping theorem, and Newton iteration, based upon the Newton-Kantorovich theorem.

4 Estimation of the Error for Picard Iteration

We begin with the specific estimation of quantities referenced in Theorem 4.

4.1 The Differentiability of T

Lemma 5. *For each $\psi_* \in \mathcal{U}$, the Fréchet derivative of T exists as a bounded linear operator $T'(\psi_*) : H_0^2 \mapsto H_0^2$ and is given by (4.1) below. The inverse operator $[I - T'(\psi_*)]^{-1}$ can be represented by a Neumann series, $\sum_{j=0}^{\infty}[T'(\psi_*)]^j$, with*

$$\kappa = \|[I - T'(\psi_*)]^{-1}\| \leq 1.56827.$$

Moreover, an estimate for the global Lipschitz constant of T' is given by

$$\|T'(u) - T'(v)\| \leq \lambda \|u - v\|_{H^2}, \ \lambda = .28089.$$

Proof. For basic facts about Neumann series, we refer to [23, p. 69]. In order to calculate the operator $T'(\psi_*)$, we use the previously mentioned fact that C^1-Fréchet differentiability is equivalent to C^1-Gateaux differentiability. Thus, by simple directional derivative arguments, we compute, for $\psi \in H_0^2$,

$$T'(\psi_*)[\psi] = \frac{1}{2} \lim_{\epsilon \to 0} \int_0^L G(\cdot\,, s) \left\{ \frac{\cos \circ (\psi_*(s) + \epsilon\psi(s)) - \cos \circ \psi_*(s)}{\epsilon} \right\} \, ds$$

$$= -\frac{1}{2} \int_0^L G(\cdot\,, s) \sin \circ \psi_*(s) \psi(s) \, ds. \tag{4.1}$$

Implicit in this calculation is the interchange of limit operations (differentiation and integration), permitted by the uniform convergence of the difference quotients. One uses the bound for $\|\mathcal{G}\|$ and the natural bound $|\sin| \leq 1$, to obtain, for $\psi \in H_0^2$,

$$\|T'(\psi_*)[\psi]\|_{H^2} \leq \frac{1}{2}\|\psi\|_2 \leq C\|\psi\|_{H^2}.$$

We thus obtain the expression,

$$\|T'(\psi_*)\| \leq .362354.$$

This could have been predicted from the contraction constant estimate for T in (2.8), which provides an independent proof. This gives the existence of the Neumann series for $[I - T'(\psi_*)]^{-1}$ as a bounded linear inverse operator, and the bound,

$$\kappa \leq \frac{1}{1 - .362354} = 1.56827.$$

The estimation of λ is as follows. For $\psi \in H_0^2$, and $u, v \in \mathcal{U}$,

$$\|[T'(u) - T'(v)][\psi]\|_{H^2} \leq \frac{1}{2}\|[\sin \circ u - \sin \circ v]\psi\|_2 \leq C \max_{0 \leq t \leq L} |u(t) - v(t)| \|\psi\|_{H^2}.$$

To bound the latter, we use the representation (2.5):

$$\max_{0 \leq t \leq L} |u(t) - v(t)| \leq \left\{ \int_0^L \max_{0 \leq t \leq L} |G(t,s)|^2 \; ds \right\}^{1/2} \|u - v\|_{H^2}.$$

Now the first factor is estimated from above by .775181 since

$$\max_{0 \leq s \leq L} G(t,s) = G(s,s) = \frac{s}{L}\left(L - s\right),$$

so that we obtain the estimate $\lambda = (.362354)(.775181) = .28089$. $\square$

4.2 Estimation of the Residual

The following lemma addresses the estimation of the individual terms in (3.6).

Lemma 6. *The contraction constant for T_N on $\mathcal{U}_N$ is given by*

$$C_h = \frac{1}{2}\left(.724708 + h^2/\pi^2\right). \tag{4.2}$$

Thus, the following hold.

i) For $n \geq 1$ we have the estimate:

$$\|\psi_n - T_N\psi_n\|_{H^2} \leq C_h^n \|\psi_1 - \psi_0\|_{H^2} \leq \frac{\|\cos\circ\psi_0\|_2}{2} C_h^n = .572501 C_h^n.$$

ii) An estimate for (3.6) is given by

$$\|\psi_n - T\psi_n\|_{H^2} \leq .572501\ C_h^n + .448265\ h^2. \tag{4.3}$$

Proof. Let ϕ, ψ be given in $\mathcal{U}_N$. Direct representation gives

$$T_N\phi - T_N\psi = \frac{1}{2}\mathcal{G}\circ I_N(\cos\circ\phi - \cos\circ\psi),$$

so that, upon taking second derivatives, and estimating the L_2 norm, we have

$$\|T_N\phi - T_N\psi\|_{H^2} = \frac{1}{2}\|I_N(\cos\circ\phi - \cos\circ\psi)\|_2 \leq \frac{1}{2}\|I_N(\phi - \psi)\|_2,$$

where the final step employs the inequality,

$$|I_N(\cos\circ\phi - \cos\circ\psi)| \leq |I_N(\phi - \psi)|.$$

This makes use of the positivity of the operator I_N and the domination of the difference of cosines by the difference $\phi - \psi$. Denoting the latter function by ω, and using the interpolation error estimates derived in [21, Theorem 1.3, p. 45] for estimating $\|\omega - I_N\omega\|_2$, we obtain, after addition and subtraction of ω:

$$\|I_N\omega\|_2 \leq \|\omega - I_N\omega\|_2 + \|\omega\|_2 \leq \left(\frac{h^2}{\pi^2}\right)\|\omega''\|_2 + \|\omega\|_2.$$

The use of (2.5) in the second term gives a contraction constant in the $H^2(0, L)$-norm bounded by

$$C_h = \frac{1}{2}\left(.724708 + \frac{h^2}{\pi^2}\right). \tag{4.4}$$

Part i) follows when the process is carried out inductively. Note that we use the estimate

$$\|\psi_1 - \psi_0\|_{H^2} = \|\cos \circ \psi_0\|_2 = 1.145.$$

The first term in (3.6) is estimated by the result of part i). The second term in (3.6) is written:

$$(T - T_N)\psi_n = \left[\frac{1}{2}\mathcal{G} \cos \circ \psi_n - \frac{1}{2}\mathcal{G} \circ I_N \cos \circ \psi_n\right].$$

This expression is estimated from above by $(\frac{h^2}{2\pi^2})\|\frac{d^2}{ds^2} \cos \circ \psi_n\|_2$, as a direct application of the error estimates for interpolation of the function $\cos \circ \psi_n$ [21, p. 45]. Differentiation of $\cos \circ \psi_n$ and use of the triangle inequality yield $\|\frac{d^2}{ds^2} \cos \circ \psi_n\|_2 \leq \|[\psi_n']^2\|_2 + \|\psi_n''\|_2$. By differentiation of the Green's function and use of the Schwarz inequality, we obtain the uniform upper bound:

$$|\psi_n'(t)| \leq \frac{\pi}{2L} + \sqrt{L/3}\|\psi_n''\|_2, \ 0 \leq t \leq L.$$

Since $\|\psi_n''\|_2 \leq \sqrt{L}$, we obtain the second term of (4.3), which yields the lemma. $\square$

4.3 The 'A Priori' Estimate

We are now able to calculate ϵ in Theorem 4. We use the upper bound $\epsilon \leq 4\kappa^2\lambda\cdot$ residual, where the residual is estimated by (3.6), and κ, λ are estimated by Lemma 5. We find that the iteration index n can be selected to be 3, as is the case when the iteration integrals are computed exactly. The minimal value of $N + 1$ required is then 10 (recall that $h = L/(N + 1)$). We obtain for these choices:

$$\|\psi_3 - T\psi_3\|_{H^2} \leq .0280311 + .0308191 = .0588501, \tag{4.5}$$

where the two balanced terms appearing in (3.6) have been displayed. We then obtain:

$$\epsilon \leq .162624, \ \delta \leq .0963852 < .1.$$

The interpretation is as follows. The 'computable' approximation ψ_3 is strictly within a tolerance of .1 of the solution θ of the pendulum equation, as measured in the H^2 norm. This estimate does *not* require knowledge of θ itself. We then have the following.

Theorem 7. *The computable sequence defined recursively for $s \in [0, L]$ by $\psi_0(s) = -\frac{\pi s}{2L}$, and*

$$\psi_n(t) = \frac{1}{2}\int_0^L G(t,s) I_N \cos \circ \psi_{n-1}(s) \, ds + \psi_0(t), \ n \geq 1,$$

converges to θ according to Theorem 4. In particular,

$$\|\psi_3 - \theta\|_{H^2} \leq .0963852$$

for $N + 1 = 10$. The iteration and discretization terms are described by (4.5) above, and this is optimal for (3.6) if $n = 3$; $\delta > .1$ if $N + 1 \leq 9$. The asymptotic value of δ, as $h \to 0$, predicted by these estimates is $\delta = .0435521$ for $n = 3$. This should be compared with the estimate of $\|\theta_3 - \theta\|_{H^2} \leq .0427165$ obtained earlier for the exact iterate θ_3.

5 Newton-Kantorovich Iteration

In the preceding, we have attempted to approximate the fixed point of T_N by 'Picard iteration', based upon the contraction mapping theorem. In this section, we shall illustrate the use of Newton-Kantorovich iteration in conjunction with Theorem 4. The Fréchet derivative of T_N is given by, where $\psi_* \in \mathcal{U}_N$:

$$T_N'(\psi_*)[\psi] = \frac{1}{2}\lim_{\epsilon \to 0}\int_0^L G(\cdot\,, s) I_N \left\{ \frac{\cos \circ(\psi_*(s) + \epsilon\psi(s)) - \cos \circ \psi_*(s)}{\epsilon} \right\} \, ds$$

$$= -\frac{1}{2}\int_0^L G(\cdot\,, s) I_N \{\sin \circ \psi_*(s)\psi(s)\} \, ds.$$

This can be seen by noting the uniform convergence of the difference quotients defining the Gateaux derivative, which coincides here with the Fréchet derivative. Integration and interpolation are continuous with respect to uniform convergence, permitting interchange of the limit with these operations. Note that the difference quotient can be written,

$$\left\{\frac{\cos\circ(\psi_*(s)+\epsilon\psi(s))-\cos\circ\psi_*(s)}{\epsilon}\right\} = -\{\sin\circ(\psi_*(s)+\epsilon_0\psi(s))\psi(s)\}$$

where ϵ_0 is selected by the mean value theorem to belong to the open interval with endpoints 0 and ϵ. This makes the stated (derivative) evaluation clear. We will interpret this map as the extended map with domain and range given by:

$$T'_N(\psi_*) : H_0^2(0,L) \mapsto \mathcal{S} \ \subset H_0^2(0,L).$$

Here, $\mathcal{S}$ is the C^2 cubic spline subspace defined in (2.12). It is customary to introduce the mapping, $F_N(u) = u - T_N(u) = (I - T_N)(u)$, so that we are attempting to determine a zero of F_N. This is analogous to the approach of §3.2. We shall suppress the dependence on N in characterizing the exact Newton iterates $\{u_n\}$, which satisfy the following characterization:

$$u_n - u_{n-1} = -[F'_N(u_{n-1})]^{-1}\ F_N(u_{n-1}), \tag{5.1}$$

in integral equation format. Since this is not solvable in a closed form which would allow for exact computation, approximation methods are required. Therefore, we shall use an operator approximation method, whereby $[F'_N(u_{n-1})]^{-1}$ is approximated by a finite truncated Neumann series:

$$[F'_N(u_{n-1})]^{-1} \mapsto \sum_{j=0}^{j=J}[T'_N(u_{n-1})]^j.$$

The new definition, characterizing the *approximate* Newton method

$$u_n - u_{n-1} = -\sum_{j=0}^{j=J}[T'_N(u_{n-1})]^j\ F_N(u_{n-1}), \tag{5.2}$$

yields an exactly computable (by *Mathematica*, for example) sequence. Here, J is an integer to be determined. It is nontrivial, however, to estimate the residual term, i. e., $\|u_n - T_N u_n\|_2$, which is the first term in (3.6). Theorems in the literature tend to estimate error for the *exact* Newton method (see [8]). The first author has shown that the Newton-Kantorovich theorem has an analog for approximate Newton methods in which the derivative inverse is approximated as above. We have not found this estimate in the form required here in any of the excellent references which have appeared since the 1980s, such as [5], [19], and [6]. We quote the result for a general mapping F, in terms of the residual decrease of the iterates. We omit the estimates for the convergence of the sequence itself. The following is a restatement of results in [9, Lemma 2.2 (esp. (2.11a)) and Theorem 2.3].

Theorem 8. *Let F be a mapping defined on a closed ball $B_r = \{x : \|x - x_0\| \le r\}$ in a Banach space X with range in a Banach space Z. We assume the following.*

Derivative Lipschitz continuity *F' exists and has a Lipschitz constant λ on B_r.*

Approximation of the identity *There is an approximation subspace Y of X and there are operators $\{\Gamma(u) : u \in B_r \cap Y\} \subset L(Z, Y)$, such that*

$$\|I - F'(u)\Gamma(u)\| \le M\|F(u)\|, \;\; u \in B_r \cap Y.$$

The operators $\Gamma(u)$ are approximate right inverses of $F'(u)$.

Boundedness of approximate derivative inverses *It is assumed that*

$$\|\Gamma(u)\| \le \kappa, \; u \in B_r \cap Y.$$

Now suppose a 'starting guess' $u_0 \in B_{\alpha r}, 0 \le \alpha < 1$, is given. If $\|F(u_0)\| \le \rho^{-1}$, and H is defined by

$$H = (2M + \lambda\kappa^2)\rho^{-1},$$

suppose that

$$H \leq \frac{1}{2}, \quad \frac{\kappa(1-\sqrt{1-2H})}{2M+\lambda\kappa^2} \leq (1-\alpha)r.$$

Then the approximate Newton sequence defined by

$$u_n - u_{n-1} = -\Gamma(u_{n-1})F(u_{n-1}),\ n \geq 1,$$

is well defined and is residually quadratically convergent in the following sense:

$$\|F(u_n)\| \leq \frac{\Theta_n}{H\rho}\left(\prod_{j=0}^{n} \tau_j^{2^{n-j}}\right)\frac{(1-\sqrt{1-2H})^{2^n}}{2^n} \tag{5.3}$$

Here, $\{\Theta_n\}$ *and* $\{\tau_n\}$ *are decreasing sequences bounded by one, and explicitly given by*

$$\Theta_0 = 1,\ \Theta_{k+1} = \frac{\Theta_k^2}{2^k\sqrt{1-2H} + \Theta_k(1-\sqrt{1-2H})^{2^k}},\ k \geq 1.$$

$$\tau_k = \sqrt{1-2H} + \frac{\Theta_k(1-\sqrt{1-2H})^{2^k}}{2^k},\ k \geq 0.$$

A more complete description, including the convergence of $\{u_n\}$, can be found in [9], although with modified notation. We will simply use the bound of unity for the parameters Θ_k, τ_k.

5.1 Estimation of the Newton-Kantorovich Parameters

We set $F(u) = (I - T_N)(u)$. In order to fit F within the framework of the previous theorem, we identify F with

$$F_0(u+\psi_0) = F(u),\ u \in \mathcal{U}_N,\ \psi_0(s) = -\pi s/(2L).$$

For F_0, we select $X = Z = H_0^2,\ Y = \mathcal{S}$. We shall not explicitly refer to F_0. Its mention is simply to create a theoretical bridge to Theorem 8.

Proposition 9. *For $\psi_* \in \mathcal{U}_N$, set*

$$\beta = \|[T'_N(\psi_*)]\|_{H^2},$$

where the operator norm is taken on H^2_0. Then we have the estimate, independent of ψ_*,

$$\beta \leq \frac{1}{2}\left(.724708 + \frac{h^2}{\pi^2}\right).$$

The upper bound is recognized as the contraction constant C_h for T_N on H^2_0 identified in (4.4). Similarly, we also have the estimate, for $u, v \in \mathcal{U}_N$,

$$\|T'_N(u) - T'_N(v)\| \leq \lambda \|u - v\|_{H^2},$$

where $\lambda = .775181\,\beta$. Also,

$$\|[I - T'_N(\psi_*)]^{-1}\| \leq \kappa := \sum_{j=0}^{\infty} \beta^j = \frac{1}{1-\beta}$$

If we define

$$\Gamma(\psi_*) = \sum_{j=0}^{j=J} [T'_N(\psi_*)]^j,$$

where $J \geq 1$, then $\|\Gamma(\psi_*)\| \leq \frac{1}{1-\beta}$, and

$$\|I - (I - T'_N(\psi_*))\Gamma(\psi_*)\| \leq \beta^{J+1}.$$

This means that $M = 1$, and J is selected such that $\beta^{J+1} \leq \|F(u_{n-1})\|_{H^2}$.

Proof. By direct estimation, for $\psi \in H^2_0$,

$$\|T'_N(\psi_*)[\psi]\|_{H^2} = \frac{1}{2}\left\|\int_0^L G(\cdot\,, s) I_N\{\sin \circ \psi_*(s)\psi(s)\}\, ds\right\|_{H^2} \leq \frac{1}{2}\|I_N \psi\|_2,$$

where we have noted that the H^2-norm evaluation is achieved by applying the L_2 norm to the twice differentiated integral expression, and have employed the positivity of the operator I_N. The remainder of the argument for β follows the corresponding argument for C_h in the proof of Lemma 6. In order to estimate λ, we write

$$\|[T_N'(u) - T_N'(v)][\psi]\|_{H^2} \leq \frac{1}{2}\|I_N\{[\sin\circ u - \sin\circ v]\psi\}\|_2 \leq \frac{1}{2}\max_{0\leq s\leq L}|u(s) - v(s)|\|I_N\psi\|_2.$$

We may use the analysis of §4.1 to estimate the maximum, and the above analysis to identify the other factor with β. We then estimate

$$\|\Gamma(\psi_*)\| \leq \sum_{j=0}^{j=J}\|[T_N'(\psi_*)]^j\| \leq \sum_{j=0}^{\infty}\beta^j.$$

□

5.2 The Residual Estimate for T_N

We are now prepared to apply Theorem 8 to estimate the residual $\|u_n - T_N(u_n)\|_{H^2}$. The stipulation that $H \leq 1/2$ suggests that we choose as our starting 'guess' the second iterate defined by successive approximation: $u_0 := \psi_2$. Direct calculation with $N + 1 = 10$ gives, via (i) of Lemma 6:

$$\beta = .365837,\ \rho^{-1} = .572501\ \beta^2 = .0766217.$$

We then calculate, with the aid of Proposition 9,

$$H = (2 + \lambda\kappa^2)\rho^{-1} = .207274.$$

The error estimate (5.3) then yields for $n = 1$:

$$\|u_1 - T_N u_1\|_{H^2} \leq .0101945.$$

5.3 The 'A Priori' Estimate

We are now prepared to apply Theorem 4. The residual estimate for T uses the triangle inequality:

$$\|u_1 - Tu_1\|_{H^2} \leq .0101945 + .0308191 = .0410136.$$

We compute from Theorem 4:

$$\delta \leq .0662541$$

which is a better approximation than the third iterate computed by Picard iteration (cf. Theorem 7). Note that J must be selected so that $J \geq 2$, since

$$\beta^{J+1} \leq \rho^{-1}.$$

Corollary 10. *If (5.2) is applied with $J = 2$ and $u_0 = \psi_2$, then the computed approximation u_1 satisfies $\|\theta - u_1\|_{H^2} \leq .0662541$.*

Appendix

A The Elastica Critical Point Formulation

In the solution to the pendulum equation (2.2), set $t = \sqrt{2}\, K_m s$ so that

$$\tilde{\theta}(s) = -\tfrac{\pi}{2} - 2\arcsin[\sqrt{m}\ \mathrm{sn}(K_m(s-1); m)],\ 0 \leq s \leq 1,$$

and $\tilde{\theta}''(s) = -K_m^2 \cos\tilde{\theta}(s)$. Let H be the Sobolev space $H^1(0,1)$ with inner product so that $\|\psi\|^2 = \psi^2(0) + \int_0^1 \dot{\psi}^2(s)ds$. Let

$$\Omega_h = \left\{ \psi \in H : \psi(0) = 0,\ \psi(1) = -\tfrac{\pi}{2},\ G(\psi) := \int_0^1 \sin\psi(s)ds = h \right\},$$

and search for critical points of $F : H \to \mathbb{R}$, restricted to Ω_h, with $F(\psi) = \frac{1}{2}\int_0^1 \dot{\psi}^2(s)ds$. The gradients in H are given by

$$\nabla F(\psi) = \psi,\ \ \nabla G(\psi) = -\int_0^s \int_0^u \cos\psi(v)dv\, du + (1+s)\int_0^1 \cos\psi(u)du\,.$$

The tangential projection of $\nabla F(\psi) = \psi$ onto $T\Omega_h$ vanishes if and only if

$$\psi(s) - \lambda(-\int_0^s \int_0^u \cos\psi(v)dv\, du + (1+s)\int_0^1 \cos\psi(u)du\,) - \mu_0 - \mu_1(1+s) = 0.$$

Let $s = 0$ and conclude that $\lambda \int_0^1 \cos\psi(u)du\, + \mu_0 + \mu_1 = 0$. The equation simplifies to

$$\psi(s) + \lambda \int_0^s \int_0^u \cos\psi(v)dv\, du + s\mu_0 = 0,$$

and

$$\lambda \int_0^1 \int_0^u \cos\psi(v)dv\, du + \mu_0 = \frac{\pi}{2}.$$

Thus, ψ is regular: $\dot\psi(s) + \lambda \int_0^s \cos\psi(u)du\, + \mu_0 = 0$, so that $\dot\psi(0) = -\mu_0$, and $\ddot\psi(s) = -\lambda\cos\psi(s)$; in particular, $\ddot\psi(0) = -\lambda$. Observe that it is not assumed a priori that $\dot\psi(0) = 0$, but a careful choice of h will yield this condition. Multiply by an integrating factor to get

$$2\dot\psi(s)\ddot\psi(s) = -2\lambda\dot\psi(s)\cos\psi(s), \quad \dot\psi^2(s) = -2\lambda\sin\psi(s) + \mu_0^2.$$

Combine this with $\dddot\psi(s) = \lambda\dot\psi(s)\sin\psi(s)$ to get

$$\dddot\psi(s) + \frac{\dot\psi^3(s)}{2} - \frac{\mu_0^2}{2}\dot\psi(s) = 0.$$

One possible solution is given by $\dot\psi(s) = A\mathrm{cn}(\alpha s + \beta; m)$, where

$$A\mathrm{cn}(\beta; m) = -\mu_0, \; A\alpha\mathrm{sn}(\beta; m)\mathrm{dn}(\beta; m) = \lambda, \; A^2 = 4m\alpha^2, \; -\frac{\mu_0^2}{2} = \alpha^2(1-2m).$$

To have a critical elastic curve that matches the pendulum solution $\tilde\theta$, the following values are needed: $m = 1/2$, $\mu_0 = 0$, $\beta = -K_m$, $\alpha = K_m$, $A = -K_m\sqrt{2}$, and

$$\lambda = A\alpha\mathrm{sn}(-K_m; m)\mathrm{dn}(-K_m; m) = K_m^2.$$

Integrate $\dot\psi^2(s) = -2\lambda\sin\psi(s) + \mu_0^2$ and use the constraint $G(\psi) = h$ to get

$$\int_0^1 \dot\psi^2(s)ds = -2K_m^2 h.$$

With the help of Legendre's formula, it follows that

$$h = -\int_0^1 \mathrm{cn}^2(K_m(s-1); m)ds = -\frac{1}{K_m}\int_0^{K_m} \mathrm{cn}^2(u; m)du =$$

$$1 - \frac{2E_m(K_m)}{K_m} = -\frac{\pi}{2K_m^2} \approx -0.456947.$$

This gives the solution discussed in section 2.2.

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