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NOISE RECONSTRUCTION FOR THE INVERSE HEAT CONDUCTION PROBLEM

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Abstract—A new automatic procedure to numerically recover the sample root mean square norm of the data error for the linear inverse heat conduction problem (IHCP)—when this information is not readily available—is presented. Numerical results are described which illustrate the accuracy of the algorithm.

1. INTRODUCTION

The inverse heat conduction problem (IHCP) involves the calculation of surface heat flux and/or temperature histories from transient, measured temperatures inside solids. The inverse problem arises in a number of situations in engineering practice: quenching of solids in a fluid, measurement of aerodynamic heating in wind tunnels and rocket nozzles, design and development of calorimeters and infrared computerized axial tomography.

The IHCP is a mathematically improperly-posed problem because the solution does not depend continuously upon the data.

Regularized methods, restricting attention to those solutions satisfying certain prescribed global bounds have been proposed by Miller [1], Miller and Viano [2] and applied to the IHCP by Manselli and Miller [3], Hills and Mullholland [4], Murio [5], Tikhovov *et al.* [6], Carasso [7] and Beck and Murio [8].

What is of present interest is the fact that, for these methods, the regularization parameter is a function of an *a priori* global bound for the solution and a known bound for the data accuracy.

In the case where only an upper bound for the L_2 data error norm is known, Miller has shown (see Method 3 in Ref. [1]) that it is still possible to select the regularization parameter in a manner which is essentially optimal with respect to the given information. However, if the given upper bound for the data error norm is not sharp or is not available, as is certainly the case in several practical applications of interest, the actual selection of the regularization parameter needs further investigation.

In this paper we present an automatic procedure to approximately recover the L_2 norm of the data error, when this information is not provided, which appears to be new.

In Section 2, the one-dimensional linear IHCP is presented and in Section 3 the parameter choice criterion is discussed. The main result is introduced in Section 4, where we describe the algorithm to approximately recover the amount of noise in the data. In Section 5 a test case of a semi-infinite body exposed to a heat flux that is initially zero, has a step increase and then drops to zero is analyzed and several numerical results are presented.

2. DESCRIPTION OF THE PROBLEM

A semi-infinite slab is considered to illustrate the method. After obtaining a measured transient temperature history $f(t)$ at some interior point $x = x_0$, the boundary heat flux $q(t)$ is recovered.

Linear heat conduction with constant thermal properties is considered, and without loss of generality, the problem is normalized by using dimensionless quantities.

The problem can be described mathematically as follows. The unknown temperature $u(x, t)$

satisfies:

$$u_t = u_{xx}, \quad 0 < x < \infty, \quad t > 0; \tag{1a}$$

$$u(1, t) \approx f(t), \quad t > 0; \tag{1b}$$

$$-u_x(0, t) = q(t), \quad t > 0; \tag{1c}$$

$$u(x, 0) = 0, \quad 0 < x < \infty; \tag{1d}$$

$$u(x, t) \quad \text{bounded as} \quad x \to \infty. \tag{1e}$$

Here, t is time, x is distance measured from the heated surface and $u(x, 0)$ is the initial uniform temperature. The objective is to estimate the surface heat flux history, $q(t)$, given the interior temperature measurements at $x = 1, f(t)$.

It is well known that conditions (1) are equivalent to the Volterra integral equation of the first kind,

$$u(1, t) = \int_0^t q(s) \frac{\partial \phi(1, t - s)}{\partial t} \, \mathrm{d}s, \tag{2}$$

where $\phi(1, t)$ is the temperature response at $x = 1$ for a unit step rise of the surface heat flux at $t = 0$.

In a more abstract setting, equation (2) can be written as

$$u(1, t) = Aq(t),$$

where A is the "data operator" and we assume that the unknown function $q(t)$ and the data function $u(1, t)$ are L_2 functions on some bounded interval of interest.

It is then natural to assume that the error function $Aq(t) - f(t)$ satisfies and L_2 error bound of the form

$$\| Aq(t) - f(t) \| = \left(\int_{t_{\min}}^{t_{\max}} [Aq(t) - f(t)]^2 \, \mathrm{d}t \right)^{1/2} \leqslant \epsilon. \tag{3}$$

In order to help stabilize the inverse problem, we will hypothesize that the unknown function $q(t)$ itself satisfies an *a priori* global L_2 bound:

$$\| q(t) \| \leqslant E. \tag{4}$$

If $q(t)$ satisfies conditions (3) and (4), it also satisfies

$$\| Aq(t) - f(t) \|^2 + \left(\frac{\epsilon}{E} \right)^2 \| q(t) \|^2 \leqslant 2\epsilon^2. \tag{5}$$

The approximation for the function $q(t)$ is then chosen as to minimize

$$J_\alpha(q) = \| Aq - f \|^2 + \alpha \| q \|^2, \tag{6}$$

where

$$\alpha = \left(\frac{\epsilon}{E} \right)^2$$

is the regularization parameter.

In what follows we will indicate the unique solution for the minimization problem in equation (6) by q_α.

3. PARAMETER CHOICE CRITERION

The following two lemmas and Theorem 1 are proved, with minor modifications, by Morozov [9] and are included here for completeness. For a more recent discussion of the problem of minimizing a quadratic objective function subject to a quadratic constraint, see Gander [10].

In actual computations only ϵ, an upper bound for the L_2 norm of the data error, is given. In general, E is not known and, consequently, it is not clear how to select the regularization parameter

α. Once a particular choice criterion is applied, the solution q_α is then obtained by solving the discretized version of the normal equations

$$(A^*A + \alpha I)q_\alpha = A^*f. \tag{7}$$

We begin our discussion by studying the behavior of each of the two terms in equation (6) as a function of the regularization parameter α. If we write

$$B_\alpha = A^*A + \alpha I, \tag{8}$$

using equation (7) and the fact that B_α is positive definite and symmetric, it follows that

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\|q_\alpha\|^2 = \frac{\mathrm{d}}{\mathrm{d}\alpha}(B_\alpha^{-1}A^*f, B_\alpha^{-1}A^*f) = -2(B_\alpha^{-1}q_\alpha, q_\alpha) \leqslant 0.$$

Moreover, since by equation (7) $A^*f \neq 0$, we conclude that under this hypothesis,

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\|q_\alpha\|^2 < 0.$$

We have proved the following.

Lemma 1

Let q_α be the solution of equation (7) with $A^*f \neq 0$. Then $\|q_\alpha\|^2$ is a decreasing function of $\alpha > 0$.

Similarly, we find that

$$\begin{aligned}\|Aq_\alpha - f\|^2 &= (Aq_\alpha - f, Aq_\alpha - f)\\ &= -\alpha(B_\alpha^{-2}A^*f, A^*f) - (B_\alpha^{-1}A^*f, A^*f) + (f,f)\end{aligned}$$

and

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\alpha}\|Aq_\alpha - f\|^2 &= 2\alpha(B_\alpha^{-3}A^*f, A^*f)\\ &= 2\alpha(B_\alpha^{-1}q_\alpha, q_\alpha) \geqslant 0.\end{aligned}$$

Again, if $A^*f \neq 0$, we conclude that

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\|Aq_\alpha - f\|^2 > 0.$$

Thus, Lemma 2 follows.

Lemma 2

If q_α is the solution of equation (7) and $A^*f \neq 0$, then $\|Aq_\alpha - f\|^2$ is an increasing function of $\alpha > 0$.

When only an upper bound ϵ for the data error is known, the monotone behavior of $\|q_\alpha\|^2$ in Lemma 1 strongly suggests to study the related problem

$$\min_{\|Aq_\alpha - f\| \leqslant \epsilon} \|q_\alpha\|^2. \tag{9}$$

That is, to find the solution of the IHCP with the smallest L_2 norm for which the residual error remains below a certain given level. This approach was introduced by Miller in Ref. [1] as Method 3. It is shown in Ref. [1] that this solution is essentially optimal with respect to the given information, even though E is unknown.

The relationship between the original problem (6) and the associated problem (9) is described in the following.

Theorem 1

If $\|Aq_{\tilde{\alpha}} - f\| = \epsilon$ for some $\tilde{\alpha} > 0$ then $q_{\tilde{\alpha}}$ is the unique solution of problem (9) obtained by solving problem (6) with $\alpha = \tilde{\alpha}$.

Proof. Because of the monotone behavior of the residual (Lemma 2), the value $\tilde{\alpha}$ for which $\| Aq_{\tilde{\alpha}} - f \|^2 = \epsilon^2$ is unique. Suppose that $q_{\tilde{\alpha}}$ is not a solution of the problem (9). Then, from equation (12), there exists $q_\alpha \neq q_{\tilde{\alpha}}$ such that $\| q_\alpha \|^2 \leqslant \| q_{\tilde{\alpha}} \|^2$ and $\| Aq_\alpha - f \|^2 \leqslant \| Aq_{\tilde{\alpha}} - f \|^2$. It follows then that $\| Aq_\alpha - f \|^2 + \alpha \| q_\alpha \|^2 \leqslant \| Aq_{\tilde{\alpha}} - f \|^2 + \tilde{\alpha} \| q_{\tilde{\alpha}} \|^2$ which is impossible since $q_{\tilde{\alpha}}$ minimizes problem (6) with $\alpha = \tilde{\alpha}$.

Theorem 1 determines a particular parameter choice criterion and, at the same time, shows how the criterion uniquely characterizes the solution of the IHCP.

The following steps summarize the application of the method to the IHCP, assuming that $\alpha_{\max} = 1$ is a valid upper bound for α.

Step 1. Set $\alpha_{\min} = 0$, $\alpha_{\max} = 1$ and choose an initial value of α between $\alpha_{\min}$ and $\alpha_{\max}$.
Step 2. Compute q_α using equation (7).
Step 3. Compute the residual $\| Aq_\alpha - f \|$.
Step 4. If $\| Aq_\alpha - f \| = \epsilon \pm \eta$, where η is a given tolerance, exit.
Step 5. Update the values of $\alpha_{\min}$, $\alpha_{\max}$ and α using the bisection method.
Step 6. Return to Step 2.

The algorithm involves, in principle, the solution of several least squares problems.

Remark

The bisection method, in Step 5, is implemented as follows:

Let $F(\alpha) = \| Aq_\alpha - f \|^2 - \epsilon^2$. Then if $F(\alpha) > \eta$, we set $\alpha_{\max} = \alpha$. If $F(\alpha) < -\eta$, we set $\alpha_{\min} = \alpha$. The updated value of α is always given by $(\alpha_{\min} + \alpha_{\max})/2$.

4. NOISE RECONSTRUCTION

The noisy data function $f(t)$ can be written as $f(t) = u(1, t) + e(t)$, where $u(1, t)$ is the true data temperature at $x = 1$ and $e(t)$ is the data error function, with $\| e(t) \| = \bar{\epsilon}$. Using the parameter choice criterion of the previous section, the solution of the IHCP depends on the regularization parameter α and also on $\bar{\epsilon}$ through the r.h.s. of the canonical equations (7). We notice that α is a function of the upper bound ϵ and, consequently, we shall denote our solution q_α^ϵ instead of q_α, for $\bar{\epsilon}$ fixed. The quality of the solution q_α^ϵ depends strongly on the sharpness of the upper bound ϵ since $\tilde{\alpha}$ is chosen such that $\| Aq_\alpha^\epsilon - f \| = \epsilon$, and it is not clear how to proceed if the information about $\bar{\epsilon}$ is very poor ($\epsilon \gg \bar{\epsilon}$). In actual computations, is it possible to decide if the given upper bound ϵ for the data error is sharp or not?

We begin by rewriting problem (9) as

$$\| q_\alpha^\epsilon \|^2 = \min_{\| Aq_\alpha^\epsilon - f \| \leqslant \epsilon} \| q_\alpha^\epsilon \|^2 \tag{10}$$

and investigating how sensitive is $\| q_\alpha^\epsilon \|$ to small changes in ϵ.

From

$$\frac{\mathrm{d} \| q_\alpha^\epsilon \|^2}{\mathrm{d}\epsilon} = \frac{\mathrm{d}}{\mathrm{d}\alpha} \| q_\alpha^\epsilon \|^2 \frac{\mathrm{d}\tilde{\alpha}}{\mathrm{d}\epsilon}, \tag{11}$$

recalling that the parameter choice criterion gives

$$\epsilon^2 = (Aq_\alpha^\epsilon - f, Aq_\alpha^\epsilon - f), \tag{12}$$

it follows that

$$\begin{aligned} 2\epsilon &= \frac{\mathrm{d}\epsilon^2}{\mathrm{d}\epsilon} = \frac{\mathrm{d}}{\mathrm{d}\alpha} \| Aq_\alpha^\epsilon - f \|^2 \frac{\mathrm{d}\alpha}{\mathrm{d}\epsilon} \\ &= 2\hat{\alpha}(B_\alpha^{-1} q_\alpha^\epsilon, q_\alpha^\epsilon) \frac{\mathrm{d}\alpha}{\mathrm{d}\epsilon}, \end{aligned} \tag{13}$$

using the formulae in Lemma 2. On the other hand,

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\|q_\alpha^\epsilon\|^2\frac{\mathrm{d}\alpha}{\mathrm{d}\epsilon} = -2(B_\alpha^{-1}q_\alpha^\epsilon, q_\alpha^\epsilon)\frac{\mathrm{d}\alpha}{\mathrm{d}\epsilon} \tag{14}$$

from the computations in Lemma 1. Combining equations (13) and (14) we obtain

$$\frac{\mathrm{d}\|q_\alpha^\epsilon\|^2}{\mathrm{d}\epsilon} = -\frac{2\epsilon}{\alpha}. \tag{15}$$

If $\epsilon \gg \bar{\epsilon}$, formula (15) indicates that $\|q_\alpha^\epsilon\|$ changes little with ϵ because the constraint in equation (10) is easily satisfied. As ϵ approaches $\bar{\epsilon}$ $(\epsilon > \bar{\epsilon})$, $\|q_\alpha^\epsilon\|$ becomes more sensitive to changes in ϵ and finally, if $\epsilon < \bar{\epsilon}$, the constraint in (10) is very restrictive and $\mathrm{d}/\mathrm{d}\epsilon\,\|q_\alpha^\epsilon\|^2$ turns out to be large in magnitude. Thus, to numerically recover $\bar{\epsilon}$, the amount of noise in the data, we can proceed as follows: introduce a decreasing sequence of upper bounds $\epsilon_i = \epsilon_0/2^i$, $i = 0, 1, 2, \ldots$, with $\epsilon_0 \gg \bar{\epsilon}$, and solve the IHCP for each i (in order) using the parameter choice criterion of Section 3. At the same time, we monitor $R_i = \|q_\alpha^{\epsilon_{i+1}}\| - \|q_\alpha^{\epsilon_i}\|$ and stop when $R_i > R$, where R is some input tolerance parameter. Ideally, we should have $\epsilon_{i+1} < \bar{\epsilon} \leqslant \epsilon_i$, and we take ϵ_i as our approximation for $\bar{\epsilon}$.

In Section 5, Problem 2 shows some practical applications of this method.

5. NUMERICAL RESULTS

In Problem 1, using the algorithm described in Section 3, the approximate reconstruction of a surface heat flux $q(t)$ is investigated for a semi-infinite body which is exposed to a heat flux of value 1 between $t = 0.2$ and $t = 0.6$ and is zero at other times. The time interval of interest is [0, 1] and the solution was computed by solving the discretized version of the normal equations (7) with $\Delta t = 0.01$. Since the associated linear system is positive definite, Choleski's method was used. With $n = 1/\Delta t$, the $n \times n$ matrix approximating the operator A has entries

$$a_{ij} = \begin{cases} 0, & \text{if } i < j \\ \phi[1, (i-j+\tfrac{1}{2})\Delta t] - \phi[1, (i-j-\tfrac{1}{2})\Delta t], & \text{if } i \geqslant j, \end{cases}$$

$1 \leqslant i, j \leqslant n$, where

$$\phi(x, t) = \frac{2}{\sqrt{\pi}}\sqrt{t}\,\exp(-x^2/4t) - x\,\mathrm{erfc}(x/2\sqrt{t}),$$

and they correspond to the temperature response at $x = 1$ for a unit heat flux at $x = 0$ for $(j-\frac{1}{2})\Delta t \leqslant t < (j+\frac{1}{2})\Delta t$. The exact temperature data for the problem is $u(1, t)$ and $u(1, j\Delta t)$ is denoted u_j. The noisy data $f(t)$ is obtained by adding a random error to u_j, i.e.

$$f_j = u_j + \delta_j, \quad j = 1, 2, \ldots, n,$$

where δ_j is a Gaussian random variable of variance σ^2. The average perturbation used in these tests is for $\sigma = 0.01$ and corresponds to approximately 5% of the maximum true temperature value, which is about 0.2. The residual error was measured using the sample root mean square norm given by

$$s = \left[\frac{1}{n}\sum_{j=1}^{n} r_j^2\right]^{1/2},$$

where r_j indicates the jth component of the residual vector $Aq_\alpha - f$. Depending on the initial choice of α, convergence to the value $\tilde{\alpha}$ determined by the criterion was reached in no more than 10 iterations. With $\epsilon = \sigma$, the tolerance η, used in Step 4 of the algorithm, was set to reflect a 0.05 error in the satisfaction of the constraint.

The exact data temperature is given by $u(1, t) = \phi(1, t-0.2) - \phi(1, t-0.6)$. Independently of the initial guess, the value of $\hat{\alpha}$ is about 8×10^{-4} and the associated error norm of the solution is approx. 0.22. Figure 1 shows the solution obtained using the criterion and Table 1 illustrates the relationship between the parameter α and the approximate error norm of the solution.

In Problem 2, we attempt to numerically recover $\bar{\epsilon}$ using the method introduced in Section 4. In all cases, we consider the test problem described in Problem 1 adding to the true data vector

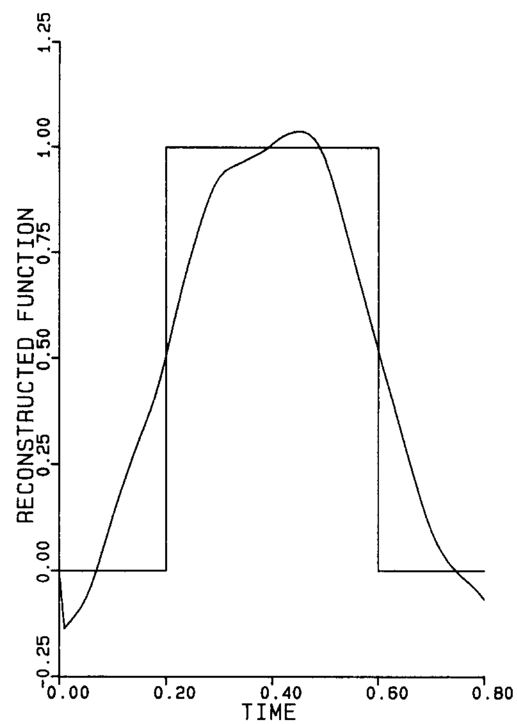

Fig. 1. Reconstructed heat flux function obtained using the parameter choice criterion with $\tilde{\alpha} \approx 8 \times 10^{-4}$.

the corresponding noise vector with $\|(\delta_1, \delta_2, \ldots, \delta_n)\| = \bar{\epsilon}$. For each $\bar{\epsilon}$, we generate a family of data vectors with the same norm by merely permuting the δ_is components. The results are summarized in Tables 2–4. The first column in these tables represent the minimum and maximum values of $\|q_\alpha^{\epsilon_i}\|$ in the family of problems, depending on the associated ϵ_i (second column) and the selected parameter $\tilde{\alpha}$ (third column).

Table 2 corresponds to the problem with error norm $\bar{\epsilon} = 5.5 \times 10^{-4}$. Our algorithm produces the approximation $\epsilon_7 \approx 3 \times 10^{-4}$.

Table 3 corresponds to the problem with $\bar{\epsilon} = 5.5 \times 10^{-3}$ and approximation $\epsilon_3 = 5 \times 10^{-3}$. This case is also illustrated in Fig. 2 for the averaged values of $\|q_\alpha^{\epsilon_i}\|$.

Finally, Table 4 corresponds to the problem with $\bar{\epsilon} = 5.5 \times 10^{-2}$ and approximation $\epsilon_1 = 5 \times 10^{-2}$.

Table 1. Error norms of the solution as a function of α

α	Error norm
10^{-7}	3.37
10^{-6}	0.912
10^{-5}	0.271
10^{-4}	0.193
10^{-3}	0.231
10^{-2}	0.366

Table 2. Norm of the solution as a function of ϵ

$\|q_\alpha^{\epsilon_i}\|$	ϵ_i	$\tilde{\alpha}$
0.331, 0.332	$\epsilon_0 = 0.04$	0.250×10^{-1}
0.425, 0.426	$\epsilon_1 = \epsilon_0/2$	0.781×10^{-1}
0.492, 0.494	$\epsilon_2 = \epsilon_0/2^2$	0.244×10^{-3}
0.541, 0.543	$\epsilon_3 = \epsilon_0/2^3$	0.839×10^{-3}
0.572, 0.575	$\epsilon_4 = \epsilon_0/2^4$	0.315×10^{-3}
0.590, 0.592	$\epsilon_5 = \epsilon_0/2^5$	0.118×10^{-3}
0.608, 0.612	$\epsilon_6 = \epsilon_0/2^6$	$0.147 \times 10^{-4}, 0.221 \times 10^{-4}$
1.410, 1.987	$\epsilon_7 = \epsilon_0/2^7$	$0.720 \times 10^{-8}, 1.44 \times 10^{-8}$
6.655, 9.438	$\epsilon_8 = \epsilon_0/2^8$	$0.113 \times 10^{-9}, 0.450 \times 10^{-9}$

Table 3. Norm of the solution as a function of ϵ

$\|q_\alpha^{\epsilon_i}\|$	ϵ_i	$\tilde{\alpha}$
0.330, 0.334	$\epsilon_0 = 0.04$	0.250×10^{-1}
0.423, 0.436	$\epsilon_1 = \epsilon_0/2$	$0.703 \times 10^{-2}, 0.781 \times 10^{-2}$
0.502, 0.517	$\epsilon_2 = \epsilon_0/2^2$	$0.176 \times 10^{-2}, 0.195 \times 10^{-2}$
0.678, 0.801	$\epsilon_3 = \epsilon_0/2^3$	$0.687 \times 10^{-5}, 1.37 \times 10^{-5}$
26.7, 35.6	$\epsilon_4 = \epsilon_0/2^4$	$0.169 \times 10^{-8}, 0.335 \times 10^{-8}$

Table 4. Norm of the solution as a function of ϵ

$\|q_\alpha^{\epsilon_i}\|$	ϵ_i	$\tilde{\alpha}$
0.098, 0.132	$\epsilon_0 = 0.1$	0.159, 0.218
0.469, 0.516	$\epsilon_1 = \epsilon_0/2$	$0.249 \times 10^{-2}, 0.341 \times 10^{-2}$
15.1, 25.0	$\epsilon_2 = \epsilon_0/2^2$	$0.381 \times 10^{-6}, 0.763 \times 10^{-6}$

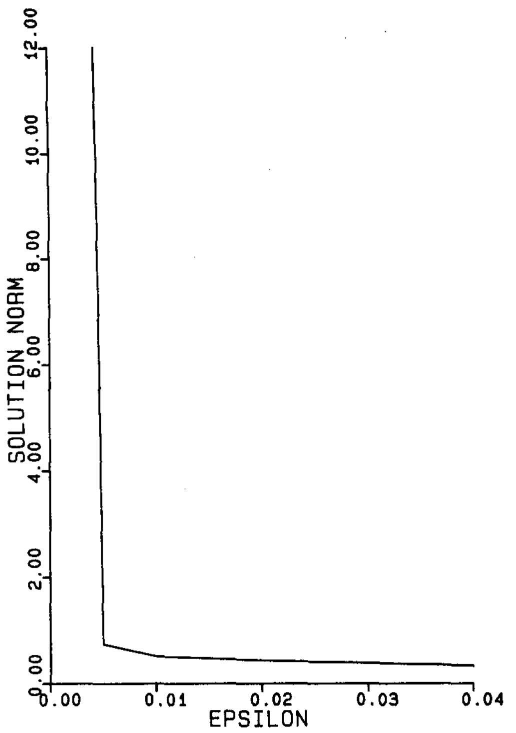

Fig. 2. Solution norm $\|q_{\bar{\epsilon}}^{\epsilon}\|$ as a function of ϵ with $\bar{\epsilon} = 5.5 \times 10^{-3}$.

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