

Numerical Approximation of Minimum Norm Solutions of $Kf = g$ for Special K

By Glenn R. Luecke

Abstract. Let $K: L_2(Y, \mu) \rightarrow L_2(X, \nu)$ be continuous and linear and assume $(Kf)(x) = \int_Y k(x, y)f(y) d\mu(y)$. Define k_x by $k_x(y) = k(x, y)$. Assume K has the property that (a) $k_x \in L_2(Y, \mu)$ for all $x \in X$ and (b) if $Kf = 0$ ν -a.e., then $(Kf)(x) = 0$ for all $x \in X$. For example, if $X = Y = [0, 1]$, $\mu = \nu$ is Lebesgue measure and if $k(x, y)$ satisfies a Lipschitz condition in x , then K has the above property. Assume K satisfies this property and f_0 is a minimum L_2 norm solution of the first-kind integral equation $(Kf)(x) = g(x)$ for all $x \in X$. It is shown that f_0 is the L_2 -norm limit of linear combinations of the k_{x_i} 's. It is then shown how to choose constants c_1, \dots, c_n to minimize $\|f_0 - \sum_{j=1}^n c_j k_{x_j}\|$ without knowing what f_0 is. This paper also contains results on how to choose the k_{x_j} 's as well as numerical examples illustrating the theory.

Introduction. Let K be a continuous linear transformation mapping $L_2(Y, \mu)$ into $L_2(X, \nu)$ defined by $(Kf)(x) = \int_Y k(x, y)f(y) d\mu(y)$; $k(x, y)$ is called the kernel of the integral operator K and is always assumed to be in $L_2(X \times Y, \nu \times \mu)$. Define k_x to be $k_x(y) = k(x, y)$. This paper considers the numerical approximation of the minimum norm solution of the first-kind integral equation $(Kf)(x) = g(x)$ for all $x \in X$ for a special class of integral operators K . For background information concerning first-kind equations, see [1].

1. Theoretical Results. The following property of the integral operator K is a key to the development of the theory.

Definition 1.1. The integral operator K with kernel function $k(x, y)$ is said to satisfy *property (C)* if

- (a) $k_x \in L_2(Y, \mu)$ for all $x \in X$, and
- (b) if $(Kf)(x) = 0$ ν -a.e. for some $f \in L_2(Y, \mu)$, then $(Kf)(x) = 0$ for all $x \in X$.

Example 1.2. Let X be an open connected set in Euclidean n -space and let ν be Lebesgue measure on X . Assume $\mu(Y) < \infty$. Assume $k_x \in L_2(Y, \mu)$ for all x and assume $k(x, y)$ is continuous in $x \in X$ uniformly in $y \in Y$, i.e., for each $x_0 \in X$ and $\varepsilon > 0$ there exists $\delta > 0$ such that if $x \in X$ such that $|x - x_0| < \delta$ then $|k(x, y) - k(x_0, y)| < \varepsilon$ for all $y \in Y$. Using the Schwarz inequality and routine real analysis, it follows that K satisfies property (C). An example of such a K is $(Kf)(x) = \int_0^1 k(x, y)f(y) dy$, $0 \leq x \leq 1$, where the partial derivative of $k(x, y)$ with respect to x is a continuous function of x and y , or if $k(x, y)$ is a continuous function of x and y satisfying the Lipschitz condition, $|k(x_1, y) - k(x_2, y)| \leq M|x_1 - x_2|^\alpha$

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for all x_1, x_2 , and y , where M and α are positive constants (independent of x_1, x_2, X, y and Y).

Let $N(K)$ denote the null space of K and let M^\perp denote the orthogonal complement of any set M , i.e., $M^\perp = \{f : (f, g) = 0 \text{ for all } g \in M\}$. Here (f, g) denotes the inner product of f and g . The goal is to find minimal hypotheses on the operator K so that $N(K)^\perp$ is equal to the L_2 -closed span of the k'_x 's, $x \in X$. For simplicity of exposition, it is assumed that all functions are real-valued.

THEOREM 1.3. *If $k_x \in L_2(Y, \mu)$ for all $x \in X$, then*

$$N(K)^\perp \subset \text{closed span}\{k_x : x \in X\}.$$

Proof. Let $M = \{k_x : x \in X\}$ and let $f_0 \in M^\perp$. Then for all $x \in X$, $(f_0, k_x) = 0$. Thus, for $x \in X$,

$$(Kf_0)(x) = \int_Y k(x, y)f_0(y) d\mu(y) = \int_Y k_x(y)f_0(y)\mu(y) = (k_x, f_0) = 0.$$

The second to last equality above is valid because it is assumed that all functions are real-valued. It follows that $f_0 \in N(K)$. Therefore, $M^\perp \subset N(K)$. Then it follows that $N(K)^\perp \subset M^{\perp\perp}$. But $M^{\perp\perp}$ is the closed span of M and the proof is complete. \square

THEOREM 1.4. *If operator K satisfies property (C), then*

$$N(K)^\perp = \text{closed span}\{k_x : x \in X\}.$$

Proof. Let $M = \text{closed span}\{k_x : x \in X\}$ and let $f_0 \in N(K)$. Then $(Kf_0)(x) = 0$ ν -a.e. Since K satisfies property (C), $(Kf_0)(x) = 0$ for all $x \in X$. Then for $x \in X$,

$$(f_0, k_x) = \int_Y k_x(y)f_0(y) d\mu(y) = \int_Y k(x, y)f_0(y) d\mu(y) = (Kf_0)(x) = 0.$$

It follows that $k_x \in N(K)^\perp$ for all $x \in X$. Thus, $M \subset N(K)^\perp$. By Theorem 1.3, $N(K)^\perp \subset M$ and hence $M = N(K)^\perp$ and the theorem is proved. \square

Recall f_0 is a minimum norm solution of $(Kf)(x) = f(x)$ if and only if $(Kf_0)(x) = g(x)$ and $f_0 \in N(K)^\perp$. Theorem 1.4 implies f_0 can be approximated as closely as desired by (finite) linear combinations of the k_x 's.

Example 1.5. To illustrate Theorem 1.4 consider the rank-2 integral operator $(Kf)(x) = \int_0^1 (x - y)f(y) dy$ mapping $L_2(0, 1)$ into $L_2(0, 1)$, Lebesgue measure. It is easy to verify that K satisfies property (C), so the hypotheses of Theorem 1.4 are satisfied. Here, $k_x(y) = x - y$, and it is easily shown that

$$\text{closed span}\{k_x : 0 \leq x \leq 1\} = \text{span}\{1, y\} = N(K)^\perp.$$

LEMMA 1.6. *Let g, h_1, h_2, \dots, h_n be elements in a Hilbert space H with the inner product of $u, v \in H$ denoted by (u, v) . Then the orthogonal projection of g onto $\text{span}\{h_1, \dots, h_n\}$ is given by $\sum_{j=1}^n a_j h_j$, where vector $(a_1, \dots, a_n)^T$ is a solution of the linear system $Ax = b$ with $a_{ij} = (h_j, h_i)$ and $b_i = (g, h_i)$.*

Proof. Let $Pg = \sum_{j=1}^n a_j h_j$ be the orthogonal projection of g onto $\text{span}\{h_1, \dots, h_n\}$. Then for each i , $g - Pg$ is perpendicular to h_i , that is,

$$0 = (g - Pg, h_i) = (g, h_i) - (Pg, h_i) = (g, h_i) - \sum_{j=1}^n (h_j, h_i)a_j.$$

From this the lemma follows. \square

Observe that the $n \times n$ matrix A in Lemma 1.6 is a Grammian matrix and hence is always nonnegative semidefinite and is positive definite if and only if $\{h_1, \dots, h_n\}$ is a linearly independent set.

The next theorem shows how to choose constants c_1, \dots, c_n so that $\sum_{j=1}^n c_j k_{x_j}$ will best approximate the minimum norm solution f_0 of $Kf = g$ in the L_2 -norm *without knowing* f_0 , that is, only $g(x)$ and the kernel $k(x, y)$ need to be known to determine the c_j 's. Most expansion methods for solving first-kind integral equations pick the constants c_1, \dots, c_n to minimize the norm of the residual instead of the norm difference from the desired solution. Let $\mathbf{c} = (c_1, c_2, \dots, c_n)^T$, $\mathbf{b} = (g(x_1), g(x_2), \dots, g(x_n))^T$, and let A be the $n \times n$ matrix whose (i, j) th component is given by (k_{x_j}, k_{x_i}) . With this notation the following theorem can be easily stated.

THEOREM 1.7. *If f_0 is the minimum norm solution of $(Kf)(x) = g(x)$, then the minimum over all constants c_1, \dots, c_n of $\|f_0 - \sum_{j=1}^n c_j k_{x_j}\|$ occurs when \mathbf{c} is a solution of $A\mathbf{x} = \mathbf{b}$. Moreover, the value of $f_n = \sum_{j=1}^n c_j k_{x_j}$ is independent of which solution \mathbf{c} of $A\mathbf{x} = \mathbf{b}$ one takes.*

Proof. By elementary properties of Hilbert spaces, $\|f_0 - \sum_{j=1}^n c_j k_{x_j}\|$ is minimized when the c_j 's are chosen so that $\sum_{j=1}^n c_j k_{x_j}$ is the orthogonal projection of f_0 onto $\text{span}\{k_{x_1}, \dots, k_{x_n}\}$. By Lemma 1.6, $\mathbf{c} = (c_1, \dots, c_n)^T$ is a solution of $A\mathbf{x} = \mathbf{b}$, where $b_i = (f_0, k_{x_i})$. But

$$(f_0, k_{x_i}) = \int_Y f_0(y) k_{x_i}(y) d\mu(y) = \int_Y k(x_i, y) f_0(y) d\mu(y) = g(x_i),$$

and the proof of the first sentence in Theorem 1.7 is complete.

Let $f_n^1 = \sum_{j=1}^n c_j k_{x_j}$ and $f_n^2 = \sum_{j=1}^n d_j k_{x_j}$, where \mathbf{c} and \mathbf{d} are solutions of $A\mathbf{x} = \mathbf{b}$. Then for each $i = 1, 2, \dots, n$

$$\begin{aligned} (f_n^1 - f_n^2, k_{x_i}) &= \sum_{j=1}^n c_j (k_{x_j}, k_{x_i}) - \sum_{j=1}^n d_j (k_{x_j}, k_{x_i}) \\ &= g(x_i) - g(x_i) = 0. \end{aligned}$$

Since f_n^1 and f_n^2 are in the span of k_{x_1}, \dots, k_{x_n} , it follows that $f_n^1 = f_n^2$ and the proof of Theorem 1.7 is complete. \square

The above argument does not obviously generalize to finding the least squares solution of minimum norm (see [4]) of $Kf = g$. The reason for this is that if f_0 is the least squares solution of minimum norm of $Kf = g$, then $(Kf_0)(x) = (Pg)(x)$ where Pg is the orthogonal projection of g onto the closure of the range of the operator K . Applying the same argument as in the proof of Theorem 1.7 yields that the c_j 's are a solution of $A\mathbf{x} = \mathbf{b}$ where A is as defined immediately preceding Theorem 1.7, but b_i now is $(Pg)(x_i)$, which is unknown.

Notice that in Theorem 1.7, the vector formed from the c_j 's can be any solution of $A\mathbf{x} = \mathbf{b}$. If the k_{x_j} 's are linearly dependent, then A will be a singular matrix. From an application point of view, it is desirable for the k_{x_j} 's to be linearly independent so that A will be positive definite and $A\mathbf{x} = \mathbf{b}$ can be solved numerically using the Cholesky decomposition.

Example 1.8. If x_1, \dots, x_n are distinct numbers in the interval $[a, b]$, then $\{e^{x_1 y}, \dots, e^{x_n y}\}$, $\{\cos(x_1 y), \dots, \cos(x_n y)\}$, and $\{\sin(x_1 y), \dots, \sin(x_n y)\}$, $x_j \neq 0$, are linearly independent sets in $L_2(a, b)$, Lebesgue measure.

Suppose $c_1 e^{x_1 y} + \dots + c_n e^{x_n y} = 0$ for all $y \in [a, b]$. Differentiate this equation i times with respect to y , $i = 1, 2, \dots, n-1$, to obtain a system of n linear equations which can be written in the form $A\mathbf{x} = 0$, where A is a Vandermonde matrix and the i th component of \mathbf{x} is $c_i e^{x_i y}$. It follows that each $c_i = 0$. The remaining two sets of functions are shown to be linearly independent in a similar fashion except the original equation should be differentiated $4, 8, 12, \dots, 4(n-1)$ times instead of $1, 2, 3, \dots, (n-1)$ times with respect to y .

A question of practical importance is: For a given value of n , how should x_1, \dots, x_n be chosen so that $\sum_{j=1}^n c_j k_{x_j}$ can best approximate the minimum norm solution, f_0 , of the integral equation $Kf = g$? Consider the case $n = 1$. Applying Theorem 1.7 to the case $n = 1$, one obtains that

$$f_1(y) = \frac{g(x_1)}{(k_{x_1}, k_{x_1})} k_{x_1}(y)$$

is the best L_1 -norm approximation to $f_0(y)$ for a given value x_1 , assuming $k_{x_1} \neq 0$, hence $(k_{x_1}, k_{x_1}) = \|k_{x_1}\|^2 > 0$. Therefore, we want to determine the value of x_1 which will minimize

$$\left\| f_0 - \frac{g(x_1)}{(k_{x_1}, k_{x_1})} k_{x_1} \right\|.$$

Using the fact that $(f_0, k_{x_1}) = g(x_1)$, one obtains

$$\left\| f_0 - \frac{g(x_1)}{(k_{x_1}, k_{x_1})} k_{x_1} \right\|^2 = \|f_0\|^2 - \frac{2g(x_1)^2}{\|k_{x_1}\|^2} + \frac{g(x_1)^2}{\|k_{x_1}\|^2} = \|f_0\|^2 - \frac{g(x_1)^2}{\|k_{x_1}\|^2}.$$

Notice that $\|f_0\|^2$ being unknown does not hamper solving this minimization problem; find the value of x_1 that maximizes $g(x_1)^2/\|k_{x_1}\|^2$. Example 1.5 is simple enough that one can calculate this value of x_1 exactly. For example, the minimum norm solution of

$$\int_0^1 (x-y)f(y)dy = 5x-3, \quad 0 \leq x \leq 1,$$

if $f_0(y) = 2 + 6y$. Using differential calculus, one can show that the maximum of $g(x)^2/\|k_x\|^2$, $0 \leq x \leq 1$, occurs when $x = 0$. Thus, the best approximation of $f_0(y)$ by functions of the form $(g(x)/\|k_x\|^2)k_x(y)$ is $(g(0)/\|k_0\|^2)k_0(y) = 9y$. Then $\|f_0\| = \sqrt{28}$ and $\|f_0 - f_1\| = 1$.

Consider $f_n = \sum_{j=1}^n c_j k_{x_j}$ for $n > 0$, \mathbf{c} a solution of $A\mathbf{x} = \mathbf{b}$ and f_0 the minimum norm solution of $Kf = g$. Since f_n is the orthogonal projection of f_0 onto $M_n \equiv \text{span}\{k_{x_1}, \dots, k_{x_n}\}$, $(f_0 - f_n, f_n) = 0$ and $(f_n, f_0) = \|f_n\|^2$. Then,

$$\begin{aligned} \|f_0 - f_n\|^2 &= (f_0 - f_n, f_0) - (f_0 - f_n, f_n) \\ &= (f_0 - f_n, f_0) = \|f_0\|^2 - (f_n, f_0) \\ &= \|f_0\|^2 - \sum_{j=1}^n c_j (k_{x_j}, f_0) = \|f_0\|^2 - \sum_{j=1}^n c_j g(x_j). \end{aligned}$$

This proves the following:

THEOREM 1.9. *To minimize $\|f_0 - \sum_{j=1}^n c_j k_{x_j}\|$ over all c_1, \dots, c_n and x_1, \dots, x_n , one need only solve: maximize $\sum_{j=1}^n c_j g(x_j)$ subject to $A\mathbf{c} = \mathbf{b}$ over all x_1, \dots, x_n .*

2. Numerical Results. All computer runs were done in double precision on a National Advanced Systems AS/9160 using the VS-FORTRAN version 1.41 compiler (with optimization level = 0) and using the MVS/XA operating system. Double-precision arithmetic on this machine means about 15 decimal digits of accuracy. The parameter N is the number of basis functions, k_{x_j} 's, that were used. The $N \times N$ linear system $A\mathbf{x} = \mathbf{b}$, see Theorem 1.7 for notation, can be singular. By Theorem 1.7, it does not matter which solution of $A\mathbf{x} = \mathbf{b}$ is used. Since A can be singular, $A\mathbf{x} = \mathbf{b}$ was numerically solved by computing the singular value decomposition of A (with the LINPACK routine DSVDC) and then computing the minimum norm solution. Owing to the finite precision of the computer's arithmetic, some computed singular values may be small instead of zero. Computed singular values that gave the smallest residual, $\|\mathbf{b} - A\mathbf{x}\|$, were used. E04JAF from the Numerical Algorithms Group (NAG) Library was used to maximize $\sum_{j=1}^n c_j g(x_j)$ subject to $A\mathbf{c} = \mathbf{b}$. All integral equations tested were of the form $\int_0^1 k(x, y)f(y)dy = g(x)$, $0 \leq x \leq 1$. Therefore,

$$a_{ij} = (k_{x_j}, k_{x_i}) = \int_0^1 k(x_j, y)k(x_i, y) dy.$$

For all numerical examples tested, this integral was evaluated exactly and no quadrature method was needed. For the purpose of evaluating the algorithm, the minimum norm solution, $f_0(y)$, was entered into the program as a function statement and $b_i = g(x_i)$ was calculated by evaluating

$$g(x_i) = \int_0^1 k(x_i, y)f(y) dy$$

exactly, where $f(y)$ is some given function used to determine $g(x)$ and may be different from $f_0(y)$.

Once the c_1, \dots, c_n had been calculated by solving $A\mathbf{x} = \mathbf{b}$, the error between the minimum norm solution $f_0(y)$ and the approximate solution,

$$f_n(y) = \sum_{j=1}^n c_j k_{x_j}(y),$$

was approximated by calculating $f_0(y) - f_n(y)$ for $y \in S$ where $S = \{0.00, 0.05, 0.10, 0.15, 0.20, \dots, 1.00\}$. (Using an increment of .01 instead of .05 had little effect on the results.)

The following table lists all of the integral equations tested, along with how well the method worked. EX denotes the example number. f_0 denotes the minimum norm solution; $k(x, y)$ denotes the kernel function. $AE = \max\{|f_0(y) - f_n(y)| : y \in S\}$, an approximation to the maximum absolute error. $RE = \max\{|f_0(y) - f_n(y)|/|f_0(y)| : y \in S, f_0(y) \neq 0\}$, an approximation to the relative error. Both AE and RE are rounded to one decimal place. RES denotes the approximation to the residual given by $\max\{|(K f_n)(x) - g(x)| : x \in S\}$. N is the

number of basis functions that yielded the best number for both AE and RE (there was no ambiguity for these test problems). A listing of the FORTRAN source code is available upon request.

EX	$f(y)$	$f_0(y)$	$k(x, y)$	AE	RE	RES	N
1	$2 + 6y$	$f(y)$	$x - y$	3×10^{-15}	1×10^{-15}	1×10^{-15}	2
2	e^y	$(18 - 6e)y$ $+ (4e + 10)$	$x - y$	2×10^{-15}	1×10^{-15}	3×10^{-16}	2
3	$2 + 3y$	$f(y)$	$(x - y)^3$	3×10^{-13}	1×10^{-13}	2×10^{-14}	5
4	1	$f(y)$	$\cos(xy)$	3×10^{-12}	3×10^{-12}	1×10^{-15}	3
5	y	$f(y)$	$\sin(xy)$	8×10^{-9}	1×10^{-8}	4×10^{-15}	8
6	$(\cos y)/3$	$f(y)$	$\cos(xy)$	1×10^{-10}	7×10^{-10}	3×10^{-16}	4
7	$\cos y - .5 \cos(\frac{y}{2})$	$f(y)$	$\cos(xy)$	3×10^{-10}	3×10^{-9}	8×10^{-16}	4
8	e^y	$f(y)$	e^{xy}	1×10^{-9}	5×10^{-10}	9×10^{-16}	5
9	$y^2 + 2y - 1$	$f(y)$	$(x - y)^2$	4×10^{-15}	6×10^{-14}	2×10^{-16}	4
10	$\sin y$	$f(y)$	e^{xy}	2×10^{-6}	4×10^{-5}	8×10^{-13}	9
11	$\cos y$	$f(y)$	e^{xy}	7×10^{-6}	7×10^{-6}	1×10^{-13}	15
12	$y^2 + 1$	$f(y)$	$\cos(xy)$	2×10^{-8}	1×10^{-7}	6×10^{-13}	5
13	$\cos(2y)$	$f(y)$	$\cos(xy)$	6×10^{-5}	4×10^{-4}	2×10^{-13}	6
14	$1 - 2y$	$f(y)$	e^{xy}	5×10^{-6}	3×10^{-5}	2×10^{-12}	10
15	e^{2y}	$f(y)$	e^{xy}	4×10^{-5}	3×10^{-5}	2×10^{-12}	10
16	$\sin(2y)$	$f(y)$	$\sin(xy)$	7×10^{-6}	1×10^{-5}	2×10^{-13}	8

To give an illustration of some of the details involved, consider Example 4. (All numbers have been rounded.) For $N = 1$, the best x_0 was 0.0068. For $N = 2$, the best (x_0, x_1) was (0, 0000, 0.9392). For $N = 3$, the best (x_0, x_1, x_2) was (0.0000, 0.6530, 0.5127). The various errors and residuals were

	$N = 1$	$N = 2$	$N = 3$
AE	1.5×10^{-5}	4.4×10^{-12}	2.7×10^{-12}
RE	1.5×10^{-5}	4.4×10^{-12}	2.7×10^{-12}
RES	9.6×10^{-7}	1.2×10^{-15}	1.0×10^{-15}

3. Conclusions. An advantage of the above method is that it automatically provides a set of basis functions that span the orthogonal complement of the null space of the integral operator K . The test examples listed above confirm that this method will work well if the minimum norm solution can be well approximated by a few of the basis functions, k_x , $x \in X$; otherwise, solutions with high precision cannot be found with this method. Since the $N \times N$ matrix A used to numerically calculate the c_j 's is a Grammian matrix (with respect to a finite-dimensional weighted inner product space), A becomes numerically ill-conditioned when N is very large. Experiments with some test problems indicate that $N \geq 25$ is normally too large. A second advantage of this method is that the coefficients of the k_{x_j} 's were calculated to minimize the norm difference of the approximate solution to the minimum norm solution, instead of choosing them to minimize the residual. The third advantage of this method is that it provides a way of picking "optimal" basis functions for a fixed value of N .

When performing these tests, the minimum norm solution, f_0 , was used to determine the value of N which yielded the best approximation, f_1 , to f_0 . This was done to obtain an accurate evaluation of the method. In applications, f_0 will be unknown, but a value of N can be determined by choosing it to minimize the residual $\|Kf_1 - g\|$, or at least an approximation to it. This was done (as described in Section 2) for all examples tested.

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Department of Mathematics and Computation Center
Iowa State University
Ames, Iowa 50011
E-mail: gmgrl@isumvs.bitnet

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