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EQUATIONS WITH WEAKLY DISCONTINUOUS KERNELS

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This thesis outlines a technique for accurately approximating a linear Volterra integral operator $(K_X)(s) = \int_0^S k(s,t)x(t)dt$. An approximation, K_n , to K, the Volterra operator, is made by replacing the integral in K by a quadrature rule on [0,1] whose weights depend on s. The special case of a modified Simpson's rule is worked out in detail. Error bounds are derived for the uniform convergence of $K_n x$ to Kx when x is a continuous function.

The technique is generalized to linear Fredholm integral operators that have kernels with finite jump discontinuities along a continuous curve. Under optimum conditions on the function x and the kernel the convergence for Simpson's rule is improved from first to fourth order.

Numerical Integration of Linear Integral Equations with Weakly Discontinuous Kernels

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NUMERICAL INTEGRATION OF LINEAR INTEGRAL EQUATIONS WITH WEAKLY DISCONTINUOUS KERNELS

I. INTRODUCTION

I.l Review of Numerical Integration of Integral Equations

In this thesis we consider integral equations of the second kind only. Consider first a Fredholm equation of the form

$$x(s) - \int_{0}^{1} K(s,t)x(t)dt = f(s), 0 \le s \le 1, (1-1)$$

where K and f are given real valued functions, the domain of K is the unit square, and x is the unknown function. One technique to find an approximation, x_n , to x is to first approximate the integral with a finite sum:

$$f(s) = x_n(s) - \sum_{j=1}^{n} w_{nj} K(s, t_{nj}) x_n(t_{nj}),$$
 (1-2)

where $\{t_{nj}\}_{j=1}^{n}$ forms a partition of [0,1], and where the w_{nj} are weights that depend on n and the integration formula used. Note that for each s, equation (1-2) is an equation in the n unknowns $\{x_n(t_{nj})\}_{j=1}^{n}$. We let s take on the n values of the partition, generating a system of n equations in n unknowns. By solving the system of equations we obtain $x_n(s)$ at the partition points in [0,1]. Finally, to approximate x(s) at the remaining points in [0,1], we use equation (1-2), which thus serves as an interpolation formula.

Consider next a Volterra integral equation of the form

$$x(s) - \int_{0}^{s} K(s,t)x(t)dt = f(s), 0 \le s \le 1, (1-3)$$

where x and f are as in the Fredholm case, but now the domain of K is the triangle $0 \le t \le s$, $0 \le s \le 1$. One technique to approximate x is to first replace K with a Fredholm kernel which is identically zero for $s < t \le 1$. The resulting Fredholm equation would then be solved as above.

The difficulty with treating Volterra equations as though they are Fredholm equations is that the approximation corresponding to equation (1-2) is usually not very good; that is, to guarantee a reasonably accurate answer the number of partition points, and hence the size of the algebraic system, usually must be very large. The source of the difficulty is the discontinuity of the new kernel along the line s = t. Disposal of this difficulty is the motivation behind this thesis.

I.2 Theorems to be Used in the Thesis

In this section we develop the theorems that will be used later, so as not to interrupt the continuity of the later discussion. The first three theorems parallel the work of Milne (1949).

<u>Definition</u>. For any nonnegative integer, n, define a function G_n as follows:

$$G_{n}(t) \equiv \begin{cases} t^{n}, t > 0, \\ 0, t \leq 0. \end{cases}$$

Note that for $n \ge 1$, G_n is continuous, and for n = 0, $G_0(t)$ is discontinuous at t = 0. Two important properties of G_n are as follows:

<u>Theorem 1</u>. For $G_n(t)$ as defined above, the derivative of G_n is

$$\frac{d}{dt}G_{n}(t) = \begin{cases} nG_{n-1}(t), n \ge 1, \\ 0, n = 0, \end{cases}$$

except for the case when n = 1 with t = 0. Further, the anti-derivative of G_n is $\frac{1}{n+1}G_{n+1}$.

Proof: Differentiating formally, we have

$$\frac{d}{dt}G_{n}(t) = \begin{cases} \frac{d}{dt}(t^{n}) = nt^{n-1}, t > 0, \\ \\ \frac{d}{dt}(0) = 0, t \le 0. \end{cases}$$

This formula obviously holds except when n = 1 and t = 0, for then the difference quotient

$$\frac{1}{h}[G_n(0+h) - G_n(0)]$$

has two different limits according as $h \rightarrow 0_{-}$ or $h \rightarrow 0_{+}$. Hence, with this single exception

$$\frac{d}{dt}G_{n}(t) = nG_{n-1}(t).$$

The second part of the theorem follows directly from the proof of the first.

<u>Theorem 2</u>. Let f be a function defined on [a,b]. If the (n+1)th derivative of f exists and is integrable on [a,b], then with G_n defined as above, and for y in [a,b]

$$f(y) = f(a) + \sum_{k=1}^{n} \frac{(y-a)^{k}}{k!} f^{(k)}(a) + \frac{1}{n!} \int_{a}^{b} G_{n}(y-u) f^{(n+1)}(a) du.$$

Proof: By the fundamental theorem of integral calculus,

$$f(y) = f(a) + \int_{a}^{y} f'(u) du = f(a) + \int_{a}^{y} (y-u)^{0} f'(u) du$$

for y in [a,b]. Integration by parts n times yields

$$f(y) = f(a) + \sum_{k=1}^{n} \frac{(y-a)^{k}}{k!} f^{(k)}(a) + \int_{a}^{y} \frac{(y-u)^{n}}{n!} f^{(n+1)}(u) du.$$

From the definition of $G_n(y-u)$ we can write

$$\int_{a}^{y} (y-u)^{n} f^{(n+1)}(u) du = \int_{a}^{b} G_{n}(y-u) f^{(n+1)}(u) du,$$

since the integrand is zero for u > y. The desired result follows immediately.

When approximating a definite integral by a finite sum, one can define a remainder operator which acts on functions:

$$R(f) \equiv \int_{a}^{b} f(t) dt - \sum_{j=1}^{n} w_{nj} f(t_{nj}) \cdot$$

See, for example, Milne (1949), or Hildebrand (1956). If the integral is indefinite we do the analogous thing:

<u>Definition</u>. Let f be defined on [a,b] and let s be in [a,b]. If the integral from a to s is approximated by a finite sum with weights that are functions of s, then we define a remainder operator acting on f and s by

$$R(f,s) \equiv \int_{a}^{s} f(t) dt - \sum_{j=1}^{n} w_{nj}(s) f(t_{nj}).$$

Note that if we construct the weights so that a polynomial of degree m or less is integrated exactly, and if f is such a polynomial, then R(f,s) = 0. Further, since the integral and summation are linear operators, R will be a linear operator with respect to its first argument.

<u>Theorem 3</u>. Let R be a remainder operator such that $R(t^k,s) = 0$ for k = 0, 1, ..., m, and s in [a,b], and let $M = \sup_{a < t < b} |f^{(m+1)}(t)|$. If $f^{(m+1)}(t)$ is Riemann

integrable, then

$$R(f,s) = \frac{1}{m!} R\left[\int_{a}^{b} G_{m}(t-u) f^{(m+1)}(u) du, s \right],$$

and further,

$$|R(f,s)| \leq \frac{M}{m!} \int_{a}^{b} |R[G_{m}(t-u), s]| du,$$

where R operates on $G_{m}(t-u)$, as a function of t, and s only.

Proof: By the previous theorem, if s is in [a,b], then we have

$$f(t) = f(a) + \sum_{k=1}^{m} \frac{(t-a)^{k}}{k!} f^{(k)}(a) + \frac{1}{m!} \int_{a}^{b} G_{m}(t-u) f^{(m+1)}(u) du.$$

Letting R operate on f(t) we have

$$R(f,s) = \frac{1}{m!} R\left[\int_{a}^{b} G_{m}(t-u) f^{(m+1)}(u) du, s \right],$$

since R is linear in its first argument, and R of a polynomial of degree m or less is zero. From the definition of R we have

$$R(f,s) = \frac{1}{m!} \left\{ \int_{a}^{s} \int_{a}^{b} G_{m}(t-u) f^{(m+1)}(u) du dt - \sum_{j=1}^{n} w_{nj}(s) \int_{a}^{b} G_{m}(t_{nj}-u) f^{(m+1)}(u) du \right\}.$$

From the theorem on iterated Riemann integrals (Fulks, 1961), the order of integration may be interchanged, leading to

$$R(f,s) = \frac{1}{m!} \int_{a}^{b} \left\{ \int_{a}^{s} G_{m}(t-u) dt - \sum_{j=1}^{n} w_{nj}(s) G_{m}(t_{nj}-u) \right\} f^{(m+1)}(u) du$$
$$= \frac{1}{m!} \int_{a}^{b} R[G_{m}(t-u), s] f^{(m+1)}(u) du,$$

and the final result follows directly.

<u>Theorem 4</u>. [Weierstrass Approximation Theorem] Let f be a real valued continuous function on a compact interval [a,b]. Then, given any $\varepsilon > 0$, there is a polynomial p (which may depend on ε), such that $|f(t) - p(t)| < \varepsilon$ for every t in [a,b]. Proof: See, e.g., Goldberg (1964), page 261.

II. The Special Integration Rule and the Volterra Case

II.1 Generating a Smooth Kernel

Consider the Volterra integral equation of the second kind:

$$x(s) - \int_{0}^{s} K(s,t) x(t) dt = \int_{0}^{s} f(s), \quad 0 \le s \le 1,$$

with the kernel, K, and the known function, f, having at least r + 1 continuous derivatives on their respective (closed) domains. A Volterra equation may be thought of as a Fredholm equation with a kernel

$$N(s,t) = \begin{cases} K(s,t), & 0 \le t \le s, \\ 0, & s < t \le l. \end{cases}$$

As mentioned in I.1, the discontinuity of N along the line s = t is the principal source of difficulty when approximating the integral by a sum.

In order to eliminate the difficulty, we subtract the discontinuity as follows:

$$f(s) = x(s) - \int_{0}^{s} \{K(s,t) - K(s,s) + K(s,s)\} x(t)dt$$
$$= x(s) - \int_{0}^{1} N_{0}(s,t)x(t)dt - K(s,s) \int_{0}^{s} x(t)dt, \quad (2-1)$$

where

$$N_{0}(s,t) = \begin{cases} K(s,t) - K(s,s), & 0 \le t \le s, \\ 0, & s \le t \le 1 \end{cases}$$

is continuous across the line s = t. We can also generate a kernel, $N_1(s,t)$, which has a continuous partial derivative with respect to t across the line s = t:

$$f(s) = x(s) - \int_0^s \{K(s,t) - K(s,s) + (s-t)K^{(1)}(s,s)\} x(t)dt$$

- K(s,s) $\int_0^s x(t)dt + K^{(1)}(s,s) \int_0^s (s-t)x(t)dt$
= x(s) - $\int_0^1 N_1(s,t)x(t)dt - \sum_{\ell=0}^1 \frac{(-1)^{\ell}}{\ell!} K^{(\ell)}(s,s) \int_0^s (s-t)^{\ell} x(t)dt$

where $K^{(l)}(s,s) = \frac{\partial^{l}}{\partial t^{l}}K(s,t) \Big|_{t=s}$, with the convention that $K^{(0)}(s,s) = K(s,s)$, and where

$$N_{1}(s,t) = \begin{cases} K(s,t) - K(s,s) + (s-t)K^{(1)}(s,s), & 0 \le t \le s, \\ 0, & s \le t \le 1, \end{cases}$$

In general then, subtracting r terms of Taylor's series generates $N_r(s,t)$, a kernel with r continuous partials with respect to t across the line s = t:

$$f(s) = x(s) - \int_{0}^{1} N_{r}(s,t) x(t) dt$$

- $\sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} K^{(\ell)}(s,s) \int_{0}^{s} (s-t)^{\ell} x(t) dt,$ (2-2)

where

$$N_{r}(s,t) = \begin{cases} K(s,t) - \sum_{\ell=0}^{r} \frac{(-1)^{\ell} (s-t)^{\ell}}{\ell!} K^{(\ell)}(s,s), & 0 \le t \le s, \\ 0, & s < t \le 1. \end{cases}$$

Clearly $N_r(s,t)$ is smooth across the line s = t. If x(t) also has r continuous derivatives on [0,1], then we can accurately approximate the first integral in (2-2) by a finite sum of the form (1-2). It is easy to show that with the differentiability assumptions on K and f that x is forced to have r continuous derivatives.

We deal with the indefinite integrals in (2-2) in section II.2. Presently, we consider the choice of r -the number of terms of Taylor's series subtracted from K(s,t). Integration rules under consideration here have error bounds which depend on a derivative, (p+1)th say, of the integrand, assuming the pth derivative is continuous. Therefore, it makes sense to choose r no greater than p. For example, with Simpson's rule p = 3(Hildebrand, 1956). Of course if K and f don't have

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sufficiently many continuous derivatives, then we must choose a smaller r.

We elaborate on the above by applying a low "order" rule repeatedly n times. For fixed s the jump discontinuity of the kernel K occurs in at most one of the subintervals of application. Let $\phi(t) = K(s,t)x(t)$ for fixed s. If we apply Simpson's rule n times on [0,1], then ϕ is discontinuous on at most one subinterval. Consequently, the error will be bounded by

$$\frac{1}{n}M_0 + (n-1)\left(\frac{1}{n}\right)^5 M_4 = \frac{1}{n}[M_0 + (n-1)\left(\frac{1}{n}\right)^4 M_4],$$

where $M_0 \ll \sup_{0 < t < 1} |\phi(t)|$ and $M_4 \ll \sup_{0 < t < 1} |\phi^{iv}(t)|$. We therefore have <u>first order</u> convergence for piecewise continuous functions ϕ which have only one discontinuity. (Note: we would have kth order convergence if the error bound was divided by 2^k when n was doubled.) In the same way, if ϕ is continuous, then we would have second order convergence. The extension is obvious, for if ϕ " is continuous then we will have fourth order convergence.

For Simpson's rule (which has fourth order convergence if the integrand is sufficiently differentiable), a good choice for r in the general case is r = 2. In this case, $N_2(s,t)x(t)$ will have a continuous second derivative with respect to t, a piecewise continuous, hence bounded, third derivative with respect to t, and

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we will have fourth order convergence. Choosing r = 3, as predicted in the earlier discussion, will not give higher order convergence.

II.2 The Quadrature Rule for Indefinite Integrals

We now develop a formula to approximate the integral

$$\int_{0}^{s} (s-t)^{\ell} x(t) dt.$$

We start with a quadrature rule to approximate the integral with N_r in (2-2). This rule will be called the "regular" rule as contrasted with the "special" rule to be developed. Using the same abscissas as in the regular rule, we obtain a special rule with weights that are functions of s and l. It is necessary to use the same abscissas in both rules so that the same n unknowns,

 ${x_n(t_{nj})}^n$, arise from both approximations. Thus, when s is allowed to take on the values of the partition, as in I.1, the system of equations will be $n \times n$ and, if nonsingular, can be solved. The theory for the special Simpson's rule is developed below.

For fixed l, and for $0 \le s \le 2h$, where $h = \frac{1}{2n}$ we require

$$\int_{0}^{s} (s-t)^{\ell} x(t) dt = \sum_{i=0}^{2} w_{i}(s,\ell) x(ih) + R(x,s), \qquad (2-3)$$

where R is defined by equation (2-3). We naturally require that $w_0(2h,0) = w_2(2h,0) = \frac{h}{3}$, and that $w_1(2h,0) = \frac{4h}{3}$; that is, the special rule reduces to the regular rule for s = 2h and $\ell = 0$. To find the three weights let R(x,s) = 0, and then let x(t) be successively the functions 1, t, and t^2 . We arrive at a system of three equations whose solution is

$$w_0 \equiv w_0(s,l) = Cs^{l+1}[2s^2 - 3sh(l+3) + 2h^2(l+2)(l+3)], (2-4a)$$

$$w_1 \equiv w_1(s, l) = -4Cs^{l+2}[s - h(l+3)],$$
 (2-4b)

$$w_2 \equiv w_2(s,l) = Cs^{l+2}[2s - h(l+3)],$$
 (2-4c)

where $C = [2h^2(l+1)(l+2)(l+3)]^{-1}$. Note that by construction of the w_i , R(x,s) for a polynomial of degree two or less will be identically zero.

II.3 The Sum of the Absolute Values of the Weights

Let $V = |w_1| + |w_2| + |w_3|$. This sum will be used in II.8. It is also important in that it provides a measure of the amplification of the errors in the ordinates (Hildebrand, 1956).

From equations (2-4) note that $w_0 \ge 0$ and $w_1 \ge 0$ for s in [0,2h] and for all $l \ge 0$. For w_2 we have three cases:

$$w_{2}(s, l) \begin{cases} \geq 0, \ l = 0, \ \frac{3h}{2} \leq s \leq 2h \ (case \ 1), \\ \leq 0, \ l = 0, \ 0 \leq s \leq \frac{3h}{2} \ (case \ 2), \\ \leq 0, \ l \geq 1, \ 0 \leq s \leq 2h \ (case \ 3). \end{cases}$$

Case 1: Since $w_2 \ge 0$, $V = w_0 + w_1 + w_2 = s \le 2h$ by construction of the weights.

Case 2: Here $w_2 \leq 0$, so $V = w_0 + w_1 - w_2$ and

$$V = \frac{s}{12h^2} (-4s^2 + 6sh + 12h^2).$$

Taking the derivative of V with respect to s we have

$$V' = 1 + \frac{s}{h} - \frac{s^2}{h^2},$$

which is a parabola that is concave downward. Since V'(0) = 1 and $V'\left(\frac{3h}{2}\right) = \frac{1}{4}$, we conclude that V must be increasing throughout $[0, \frac{3h}{2}]$ so that

$$V \leq V\left(\frac{3h}{2}\right) = \frac{3h}{2} < 2h$$
.

Case 3: Again $w_2 \leq 0$, so

$$V = C[-4s^{\ell+3}+2h(\ell+3)s^{\ell+2}+2h^2(\ell+2)(\ell+3)s^{\ell+1}],$$

where $C = [2h^2(l+1)(l+2)(l+3)]^{-1}$. Taking the derivatives as in case 2, we have $V' = C(l+3)s^{l}a(s)$, where

$$a(s) = -4s^{2} + 2h(l+2)s + 2h^{2}(l+1)(l+2).$$

Since the product $C(l+3)s^{l}$ is always non-negative, the sign of V' is determined by the sign of a(s). And since a(s) is a parabola that is concave downward with a(0) > 0and a(2h) > 0, we conclude that V is increasing throughout [0,2h]. Thus,

$$V \leq V(2h) = g(l)(2h)^{l+1},$$

where

$$g(l) = \frac{l^2 + 7l + 4}{(l+1)(l+2)(l+3)}$$

for $\ell > 1$. We have thus established

Result I. The sum of the absolute values of the weights of the special Simpson's rule is given by

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 $V \leq g(l)(2h)^{l+1}$, where

$$g(\ell) \equiv \begin{cases} 1, \ \ell = 0, \\ \frac{\ell^2 + 7\ell + 4}{(\ell+1)(\ell+2)(\ell+3)}, \ \ell \geq 1. \end{cases}$$

Note that g(l) is decreasing for $l \ge 0$ so that for $l \ge 0$ the maximum of g(l) is one at l = 0. Therefore, the sum of the absolute values of the weights is bounded for all l and for all s in [0, 2h].

II.4 The Remainder for the Special Integration Rule

From equation (2-3) we have the remainder of an arbitrary function x:

$$R(\mathbf{x},\mathbf{s}) \equiv \int_{0}^{\mathbf{s}} (\mathbf{s}-\mathbf{t})^{\ell} \mathbf{x}(\mathbf{t}) d\mathbf{t} - \sum_{i=0}^{2} w_{i}(\mathbf{s},\ell) \mathbf{x}(i\mathbf{h}), \qquad (2-5)$$

where $0 \le s \le 2h$. From theorem 2 of I.3, x(t) may be written

$$x(t) = x(0) + tx'(0) + \frac{t^2}{2}x''(0) + \frac{1}{2}\int_0^{2h} G_2(t-u)x'''(u)du$$

Applying the remainder function to this equation, we have

$$R(x,s) = R\left[\frac{1}{2}\int_{0}^{2h}G_{2}(t-u)x''(u)du, s\right],$$

and applying theorem 3 we can interchange R and the integral to get

$$|R(x,s)| \leq \frac{M_3}{2} \int_0^{2h} |R[G_2(t-u), s]| du,$$
 (2-6)

where $M_3 \equiv \sup_{0 < t < 1} |x'''(s)|$.

To determine $R(G_2,s)$ apply (2-5) with x(t) replaced by $G_2(t-u)$. With $W = \sum_{i=0}^{2} w_i(s,l)G_2(ih-u)$, we have

$$R(G_2,s) = \int_0^s (s-t)^{\ell} G_2(t-u) dt - W.$$

Integrating by parts l times (using theorem 1), and then integrating G_{l+2} directly yields

$$R(G_{2},s) = -\sum_{i=0}^{\ell-1} \frac{2\ell(\ell-1)\dots(\ell-i)}{(i+2)!} x^{\ell-i}G_{i+3}(-u)$$

$$-\frac{2\ell!}{(\ell+3)!} [G_{\ell+3}(-u) - G_{\ell+3}(s-u)] - W.$$

Since $0 \le u \le 2h$, $G_n(-u) \equiv 0$, so we have

Result II. If x has a continuous second derivative and a bounded third derivative, then

$$|R(x,s)| \leq \frac{M_3}{2} \int_0^{2h} |LG_{l+3}(s-u) - \sum_{i=1}^2 w_i(s,l)G_2(ih-u)| du, \quad (2-7)$$

where $M_3 = \sup_{0 \le s \le 2h} |x'''(s)|$ and $L = 2[(l+1)(l+2)(l+3)]^{-1}$.

Analytic integration of (2-7) for arbitrary l is difficult due to the absolute value inside the integral. The case for l = 0 will be worked out below. For a general l, note that the integrand is continuous and its first derivative is piecewise continuous. Therefore, we are assured that the integral exists and can be accurately approximated by the repeated midpoint rule, say. A computer program to estimate the remainder at selected points in [0,2h] was written and is presented in Appendix A. The results for l = 0, 1, 2, and 3 are presented graphically in figure 1 on the next page.





Sketch graph of the remainder for l = 0, 1, 2, 3.

For l = 0 we have from (2-7)

$$|R(\mathbf{x},\mathbf{s})| \leq \frac{M_3}{2} \int_0^{2h} |\frac{1}{3}G_3(\mathbf{s}-\mathbf{u}) - \mathbf{w}_1(\mathbf{s},0)G_2(\mathbf{h}-\mathbf{u}) - \mathbf{w}_2(\mathbf{s},0)G_2(\mathbf{2h}-\mathbf{u})| d\mathbf{u}$$

This splits into two cases: For $0 \le s \le h$ we have

$$R(G_{2},s) = \begin{cases} -w_{2}(s,0)(2h-u)^{2}, & u \in [h,2h] \\ -w_{1}(s,0)(h-u)^{2} - w_{2}(s,0)(2h-u)^{2}, & u \in [s,h] \\ \frac{1}{3}(s-u)^{3} - w_{1}(s,0)(h-u)^{2} - w_{2}(s,0)(2h-u)^{2}, & u \in [0,s]. \end{cases}$$

And for $h < s \leq 2h$ we have

$$R(G_{2},s) = \begin{cases} -w_{2}(s,0)(2h-u)^{2}, & u \in [s,2h] \\ \frac{1}{3}(s-u)^{3} - w_{2}(s,0)(2h-u)^{2}, & u \in [h,s] \\ \frac{1}{3}(s-u)^{3} - w_{1}(s,0)(h-u)^{2} - w_{2}(s,0)(2h-u)^{2}, & u \in [0,h]. \end{cases}$$

Thus in both cases we can split the integral into three parts and deal with each part separately. By writing out $w_1(s,0)$ and $w_2(s,0)$ and noting the signs of w_1 and w_2 it can be shown (the algebra is tedious) that for $\ell = 0$

$$|R(x)| \leq \frac{M_3 h^4}{24}$$
,

for all s in [0,2h], which is what the program calculated for $\ell = 0$.

The fact that the integrand of (2-7) is continuous on [0,2h] shows that there is a number e_{ϱ} depending

on ℓ and $\sup |x'''(s)|$ for $s \in (0,2h)$ such that

$$|R(x,s)| \leq e_{\ell}h^{\ell+4};$$

that is, the bound on the remainder can be made independent of s. This fact will be used in II.7 to prove a uniform convergence theorem.

II.5 Applying the Formula

Let us reconsider the original problem:

$$f(s) = x(s) - \int_{0}^{s} K(s,t)x(t)dt, 0 \le s \le 1.$$
 (2-8)

Recall that to approximate the function x we choose an integration rule and a corresponding partition of [0,1], convert (2-8) to a Fredholm equation with a kernel N(s,t) which is zero for t > s, and approximate the Fredholm integral with a finite sum. This approximation leads to an $n \times n$ system of equations whose solution determines an approximation to x at the partition points.

Suppose we choose Simpson's rule repeated n times so that the partition is $\{ih\}_{i=0}^{2n}$, h = 1/2n. First note in (2-8) that if s = 0 then the integral is zero, so x(0) = f(0). Consequently, we assume $2jh < s \le (2j+2)h$, for some j = 0, 1, 2, ..., n-1. The Fredholm problem can then be written

$$f(s) = x(s) - \int_{0}^{2jh} K(s,t)x(t)dt - \int_{2jh}^{1} N(s,t)x(t)dt. (2-9)$$

If K and x have continuous third and bounded fourth derivatives with respect to t on [0,2jh], then we can approximate the first integral in (2-9) using the regular Simpson's rule j times:

$$\int_{0}^{2jh} K(s,t)x(t)dt \approx \frac{h^{j-1}}{3} \sum_{i=0}^{2} \{K(s,t_{2i})x_{2i} + 4K(s,t_{2i+1})x_{2i+1} + K(s,t_{2i+2})x_{2i+2}\},$$

where $x_k = x(t_k)$ and $t_k = kh$. We use the regular rule because it has a higher order remainder than the special rule and, hence, is likely to be more accurate.

Next, consider the second integral in (2-9). Since $N(s,t) \equiv 0$ for t > s, we have

$$\int_{2jh}^{l} N(s,t)x(t)dt = \int_{2jh}^{(2j+2)h} N(s,t)x(t)dt .$$

When s takes on the partition points there will be two cases: s = (2j+1)h and (2j+2)h. In the second case $N(s,t) \equiv K(s,t)$ on [2jh, (2j+2)h], so the integral can be approximated by the regular Simpson's rule applied once.

In the first case we use the results of II.1 as follows:

$$\int_{2jh}^{(2j+2)h} K(s,t)x(t)dt = \int_{2jh}^{(2j+2)h} N_{r}(s,t)x(t)dt$$
$$- \sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} K^{(\ell)}(s,s) \int_{2jh}^{s} (s-t)^{\ell}x(t)dt$$

where s = (2j+1)h. To approximate this integral use the regular rule on the integral with N_r and the special rule on the integral with $(s-t)^{\ell}$. Recalling that $N_r \equiv 0$ for $t \geq s$, and letting $K_{2j+1}^{(\ell)} = K^{(\ell)}(s_{2j+1},s_{2j+1})$, we

have

$$\int_{2jh}^{(2j+1)h} K(s,t)x(t)dt \approx \frac{h}{3}N_{r}(s,t_{2j})x_{2j}$$
$$- \sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} K_{2j+1}^{(\ell)} \left\{ \sum_{i=0}^{2} w_{i}(h,\ell)s_{2j+1} \right\}.$$

Summarizing the above work, we have three cases:

$$s = 0: \int_{0}^{s} K(s,t)x(t)dt = 0, \qquad (2-10a)$$

$$s = (2j+1)h: \int_{0}^{s} K(s,t)x(t)dt \approx \frac{h}{3} \frac{j-1}{j=0} \{K(s,t_{2i})x_{2i} + 4K(s,t_{2i+1})x_{2i+1} + K(s,t_{2i+2})x_{2i+2}\} + \frac{h}{3}N_{r}(s,t_{2j})x_{2j} - \sum_{k=0}^{r} \frac{(-1)^{k}}{k!}K_{2j+1}^{(k)} + \sum_{i=0}^{s} W_{i}(h,k)x_{2j+i}, \qquad (2-10b)$$

$$s = (2j+2)h: \int_{0}^{s} K(s,t)x(t)dt \approx \frac{h}{3} \frac{j}{i=0} \{K(s,t_{2i})x_{2i} + 4K(s,t_{2i+1})x_{2i+1} + K(s,t_{2i+2})x_{2i+2}\}. \qquad (2-10c)$$

Substituting approximations (2-10) into equation (2-8) generates a system of 2n + 1 equations in the 2n + 1 unknowns that will be of the form indicated in Figure 2. The *'s indicate generally nonzero entries. The elements inside the dashed lines are given in Figure 3. The elements are shown with a general subscript, and as indicated, the two-by-two system is repeated n times. Hence, the

$$\begin{pmatrix} \begin{bmatrix} \mathbf{x} & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x}$$

AX = F

Figure 2. A Schematic for the Array A for n = 3.

system is reducible; that is, from the zeroth equation $x_0 = f_0$. Substitution of $x_0 = f_0$ into the first through (2n)th equation reduces the system to $(2n) \times (2n)$. From equations one and two x_1 and x_2 can be found using Cramer's rule; substitution for x_1 and x_2 in equations three through 2n reduces the system to $(2n-2) \times (2n-2)$. Repeating this process on the pairs (x_3, x_4) , (x_5, x_6) ..., (x_{2n-1}, x_{2n}) will solve the system.

It is important to note that since a general formula for the elements of the system can be written, it is unnecessary to store the whole array. In fact, only the two-bytwo subsystems are stored as the elements are calculated. A computer program using Simpson's rule is presented in

row	column 2j+1	column 2j+2
0)	0	0
	• •	
2j)	0	0
2j+1)	$1 - \sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} \kappa_{2j+1}^{(\ell)} w_{1}(h,\ell)$	$-\sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} K_{2j+2}^{(\ell)} W_{2}(h,\ell)$
2j+2)	-4h K _{2j+2,2j+1}	1 - ^h K _{2j+2,2j+1}
2j+3)	-4h K _{2j+3,2j+1}	- <u>2h</u> K _{2j+3} , 2j+2 + T _{2j+3}
2j+4)	-4h K _{2j+4} ,2j+1	$-\frac{2h}{3}K_{2j+4,2j+2}$
		•
2n)	$-\frac{4h}{3} K_{2n,2j+1}$	$-\frac{2h}{3} K_{2n,2j+2}$

Column 0 is a special case:

 $A_{0,0} = 1; A_{1,0} = -\frac{h}{3}K_{1,0} + T_{1}; A_{v,0} = -\frac{h}{3}K_{v,0} v = 2,3,...,n.$

Key:
$$K_{u,v} = K(s_u, s_v), \quad s_u = uh$$

 $T_u = \sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} K_u^{(\ell)} \left| \frac{h^{\ell+1}}{3} - w_0(h, \ell) \right|$

Figure 3. General Formulas for the Elements of the Array A.

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Appendix B. When solving an actual problem, one needs the following information:

- 1) The known functions f and K, and
- The partial derivatives of K with respect to t.

These formulas are used as indicated by the <u>comment</u> statements in the program. The only inputs are n (which determines h and hence the error bound) and r (the number of terms of Taylor's series to be used).

Some examples are given in II.10.

II.6 Interpolation Using the Special Rule

Further consideration of the approximations in the previous section and the development of the special rule in II.1 and II.2 indicates that an interpolation formula may be easily obtained.

Suppose we have approximated the solution, x, at the points of some partition of [0,1]. Further, suppose that an arbitrary s is given, $0 \le s \le 1$, and the number x(s) is desired. If s = 0, then we have immediately x(0) = f(0). Consequently, assume $2jh < s \le (2j+2)h$ for some j = 0, 1, 2, ..., (n-1). As before, we arrive at equation (2-9) on page 24 but now we solve for x(s):

$$x(s) = f(s) + \int_{0}^{2jh} K(s,t)x(t)dt + \int_{2jh}^{(2j+2)h} N(s,t)x(t)dt. \quad (2-11)$$

The first of these integrals is approximated as before using the regular Simpson's rule j times. In the second integral we generate a smooth kernel as in II.5. The integral with N_r is approximated with Simpson's rule once on the interval [2jh,2jh+2h], and the integral with (s-t)^{ℓ} is approximated with the special rule. The final approximation is as follows:

$$\int_{0}^{s} K(s,t)x(t) dt \approx \frac{h}{3} \frac{j-1}{\sum_{i=0}^{r} \{K(s,t_{2i})x_{2i} + 4K(s,t_{2i+1}) + K(s,t_{2i+2})x_{2i+2}\} + \frac{h}{3}N_{r}(s,t_{2j})x_{2j} + \frac{4h}{3}N_{r}(s,t_{2j+1})x_{2j+1} + \frac{r}{2}\sum_{k=0}^{r} \frac{(-1)^{k}}{k!} K^{(k)}(s,s) \left\{ \sum_{i=0}^{2} w_{i}(s-2jh,k)x_{2j+i} \right\}.$$
(2-12)

Notice that for 2jh < s < (2j+2)h the approximation involves the previous calculated values of x up through $x_{2j+2} = x(2jh+2h)$. Hence, the formula for x(s) is not an extrapolation but an interpolation:

 $x(s) \sim f(s) + [approximation (2-12)].$

II.7 Convergence of the Approximation for Smooth Functions

We now investigate convergence of the approximations of the last two sections to their respective integrals as $n \rightarrow \infty$. Our hope, to be established in II.9, is that if these approximations converge to their integrals then the corresponding approximate solutions, x_n , will converge (in some sense) to the correct solution, x, as $n \rightarrow \infty$.

Let us fix x and choose an arbitrary s in the half-open interval (0,1]. [There is no loss of generality, for if s = 0, then x(0) = f(0) by (2-10a).] In order to investigate convergence, we write

 $E \equiv \int_0^s K(s,t)x(t)dt - [Approximation (2-12)]. \quad (2-13)$

Assume r is a non-negative integer and let p = min{3, r+1}. Assume K has p + 1 partial derivatives with respect to t and x has p + 1 derivatives. It is well-known (Hildebrand, 1956) that for each application of Simpson's rule, the error bound is $h_{p+1}^{p+2}M_{p+1}$ where in this case

$$M_{p+1} = C_{p+1} \sup_{0 < t < 1} \left| \frac{\partial^{p+1}}{\partial t^{p+1}} K(s,t) x(t) \right|.$$

If p = 3, for example, then $C_4 = 1/90$. In the first three terms of (2-12) we applied Simpson's rule j times to the integral with K(s,t)x(t) and once to the integral of $N_r(s,t)x(t)$.

$$M_{p}^{*} = C_{p} \sup_{0 < t < 1} \left| \frac{\partial^{p}}{\partial t^{p}} N_{r}(s, t) x(t) \right|,$$

then the magnitude of the error from these three terms will be bounded by

$$jM_{p+1}h^{p+2} + M_p*h^{p+1} \leq \frac{C}{n^{p+1}}$$
.

By the results of II.4, the error bound for approximation of $\int_{2jh}^{s} (s-t)^{\ell} x(t) dt$ will be less than or equal to $A_{p,\ell}h^{\ell+p+1}$, where $A_{p,\ell} = Q_{p,\ell} \sup_{0 < t < l} |x^{(p)}(t)| \cdot Q_{3,\ell}$

for example are the numbers from equation (2-7) and suggested in figure 1. Therefore,

$$|\mathbf{E}| \leq \frac{\mathbf{C}}{\mathbf{n}^{\mathbf{p+1}}} + \mathbf{h}^{\mathbf{p+1}} \sum_{\ell=0}^{\mathbf{L}} \frac{1}{\ell!} \mathbf{A}_{\mathbf{p},\ell} \mathbf{N}_{\ell} \mathbf{h}^{\ell}$$
$$= [\mathbf{C} + 2^{-\mathbf{p-1}} \sum_{\ell=0}^{\mathbf{T}} \frac{1}{\ell!} \mathbf{A}_{\mathbf{p},\ell} \mathbf{N}_{\ell} \mathbf{h}^{\ell}] \frac{1}{\mathbf{n}^{\mathbf{p+1}}}$$

where $N_{\ell} = \sup_{0 < t < 1} |K^{(\ell)}(s,s)|$. (Note that this requires $r \leq 3$.) By the above work we have established

<u>Result III</u>. If K(s,t) and its first p + 1 partial derivatives with respect to t are bounded for $0 \le t \le s$ and $0 \le s \le 1$, and if x(t) and its first p + 1 derivatives are bounded on $0 \le t \le 1$, where r is the high-

est order derivative subtracted from the kernel and $p = \min\{3, r+1\}$, then there is a constant \mathcal{M} , depending on the above bounds, such that the error in approximating

$$\int_0^s K(s,t)x(t)dt, \quad 0 < s \le 1,$$

with n applications of Simpson's rule and its modification on [0,1] is bounded by

$$|\mathbf{E}| \leq \frac{\mathcal{M}}{n^{p+1}}$$
.

That is, the approxiamtion converges uniformly to the integral as $n \rightarrow \infty$.

Note that by Result III there is no gain in taking r > 2 for the Simpson's rule case. This confirms the prediction in II.l that r = 2 is a good choice.

II.8 Convergence of the Approximation for Continuous Functions

In the previous section strong assumptions were made on the solution. Uniform convergence of the approximation operator to the integral operator can also be established if the solution, x, is only known to be continuous.

The starting point is the Weierstrass approximation theorem (see I.2 Theorem 4): given $\varepsilon > 0$, there is a polynomial q(s) such that $|q(s) - x(s)| < \varepsilon$ for every s in [0,1]. Knowing that such a polynomial exists, we look to equation (2-12). Recalling the definition of E in equation (2-13) we subtract and add q wherever x occurs. Using the associative and distributive laws and the linearity of the integral and summand, we have, for example,

$$\int_{0}^{s} K(s,t)x(t)dt = \int_{0}^{s} K(s,t)q(t)dt + \int_{0}^{s} K(s,t)[x(t) - q(t)]dt.$$

Next, we use the triangle inequality and the property of integrals $|\int \phi(t) dt| \leq \int |\phi(t)| dt$ for any integrable function ϕ , to write

$$|E| \leq \left| \int_{0}^{s} K(s,t)q(t)dt - [Approximation of K(s,t)q(t)] \right|$$

+ [The remaining terms of (2-12) with q(t)]
+ [(2-12) with $|x(t)-q(t)|$ wherever x occurs]. (2-14)

Note that the first two terms of (2-14) constitute the error in approximating the integral of K(s,t)q(t). So, by Result III, the error of this approximation is less than or equal to $\mathcal{M}_q n^{-p-1}$, for some \mathcal{M}_q depending on q. Finally, we use the assumption that $|K(s,t)| \leq M_0$, that $|x(t)-q(t)| < \varepsilon$, and that the sum of the weights of the special rule is less than or equal to $(2h)^{\ell+1}$ to assert that the sum of the absolute values of all the weights will be bounded by

$$1 + \sum_{\ell=0}^{2} (2h)^{\ell+1} \leq 2, \text{ say,}$$

for n sufficiently large, and using this to conclude that

$$|\mathbf{E}| \leq \eta \varepsilon + \eta_q n^{-p-1} \neq \eta \varepsilon$$
, as $n \neq \infty$

uniformly. Further, \mathcal{P}_{1} is independent of ε , and since ε is arbitrary $|E| \rightarrow 0$ as $n \rightarrow \infty$.

II.9 Convergence to the Solution

In II.7 and II.8 we showed that the Simpson's rule approximations converged to the integral as $n \rightarrow \infty$. Following the lead of Anselone (1965), define the operators K and K_n as follows:

$$(Kx)(s) \equiv \int_{0}^{s} K(s,t)x(t)dt$$

 $(K_n \mathbf{x})(\mathbf{s}) = [\text{the approximation } (2-12)].$

Then our results have shown that

$$K_n \mathbf{x} \rightarrow K \mathbf{x}$$
 uniformly as $n \rightarrow \infty$.

The integral equation and the approximate equation have their corresponding operator equations:

$$x - Kx = f$$
, (2-15a)
 $x_n - K_n x_n = f$. (2-15b)

Solving for x in equation (2-15a) and subtracting (2-15b) from the result we have

$$x - x_n - K_n x + K_n x_n = K x - K_n x_n$$

after subtracting $K_n x$ from both sides. This equivalent to

$$(I-K_{n})(x-x_{n}) = Kx - K_{n}x,$$

where I is the identity operator. If the operator (I-K_n) has an inverse, that is, if the determinant of the matrix A represented in Figure 2 is non-zero, then we can operate on the left by $(I-K_n)^{-1}$ to get

$$x - x_n = (I - K_n)^{-1} (Kx - K_n x),$$

and taking norms we have that

$$||x-x_n|| \le ||(1-K_n)^{-1}|| \cdot ||Kx-K_nx||$$
.

Now, if $||(I-K_n)^{-1}|| \le B$ for some B and for all n, then $||x-x_n|| \le B ||Kx-K_nx|| \to 0$ as $n \to \infty$, since $K_nx \to Kx$ uniformly as $n \to \infty$. Thus we have

$$||\mathbf{x}-\mathbf{x}_n|| \leq \overline{B} \frac{1}{n^{p+1}}$$

for some \overline{B} as defined in Result III.

Note that since K is a Volterra operator $(I-K)^{-1}$ exists and it can be shown (Anselone, 1965) that $||(I-K_n)^{-1}||$ $\rightarrow ||(I-K)^{-1}||$ for all x continuous on [0,1] as $n \rightarrow \infty$. This implies that $||(I-K_n)^{-1}|| \leq B$ for some B.

II.10 Examples

In this section we present four examples that illustrate the results predicted in section II.9. The data are presented in TABLES 1 through 4. The numbers are the maximum of the errors listed on the computer print out, and it is suggested that they "close to" the norm of the error, using the max norm. The numbers in parentheses are the convergence factors--the error at one value of n is divided by the convergence factor to obtain the error for twice the value of n. The columns are for the various values of r, with * indicating regular Simpson's rule and 0 indication that K(s,s) only was subtracted.

Examples one and two are initial value problems:

1) $x'(s) = x(s), x(0) = 1 \implies x(s) = e^{S}$.

2)
$$x'(s) - (3s^2 - 4s + 1)x(s) = 0, x(0) = 1$$

=> $x(s) = e^{s^3 - 2s^2 + s}$.

The results speak largely for themselves--using the best value for r we obtain a convergence rate of 16 just as predicted. Note also that the error with just two applications of the modified rule is many times better than the error using 32 applications of the regular rule. This suggests a significant savings in computer time to obtain a desired degree of accuracy by using the modification.

n	*		<u>0</u>	
2	0.763	(2.0)	0.000492	(12 7)
4	0.374	(2.0)	0.0000360	(13.7)
8	0.188	(2.0)	0.00000244	(14./)
16	0.0941	(2.0)	0.00000159	(15.3)
32	0.0471	(2.0)	0.000000101	(15.9)

Worst error of grid points and 0.01, 0.02, ..., 0.99, 1.0

<u>n</u>	*		<u>0</u>	
2	0.764	(2.0)	0.000497	(12.0)
4	0.375	(2.0)	0.0000361	(10.0)
8	0.188	(2.0)	0.00000244	(14./)
16	0.0941	(2.0)	0.000000159	(15.3)
32	0.0471	(2.0)	0.0000000101	(15.9)

 $x'(s) = x(s), x(0) = 0, \text{ or } x(s) - \int_{0}^{s} x(t) dt = 1.0$

TABLE 1. Example 1: A listing of the worst error at the grid points and at the points j(0.01), for j = 1, 2, ..., 100.

<u>n</u>	*	0	<u>1</u>	2	
2	0.0442	0.0332	0.00153	0.00148	(19.5)
4	0.0457	0.00992	(3.8)	0.0000756	(16, 0)
8	0.0336	0.00258	0.00000506	0.00000472	(16.1)
16	0.0190	0.000651	0.00000312	0.00000292	(15.9)
32	0.00999	0.000163	0.000000194	4 0.000000183	(10.))
		Worst of G	rid and interpolation	points	
<u>n</u>	*	<u>0</u>	<u>1</u>	<u>2</u>	
2	0.0735	0.0332	0.00403	0.00148	(19.5)
4	0.0557	0.00992	0.000394	0.0000756	(16.0)
8	0.0336	0.00258	0.0000447	0.00000472	(16 1)
16	0.0190	0.000651	0.00000536	(8.1)	(15.9)
32	0.00999	0.000163	0.00000658	0.000000183	(,

TABLE 2. Example 2:
$$x'(s) - (3s^2 - 4s + 1)x(s) = 0$$
, $x(0) = 1$ or
 $x(s) - \int_0^s (3t^2 - 4t + 1)x(t)dt = 1$. $x(s) = \exp(s^3 - 2s^2 + s)$.

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<u>n</u>	*		<u>0</u>		<u>1</u>		2	
2	0.211	(1.9)	0.0103	(2.8)	0.000404	(14.2)	0.000262	(13.7)
4	0.113	(2,0)	0.00369	(3.4)	0.0000284	(15.5)	0.0000191	(15.0)
8	0.0572	(2,0)	0.00107	(3,7)	0.0000183	(15.8)	0.00000127	(15.6)
16	0.0287	(2,0)	0.000288	(3.9)	0.00000116	(16.1)	0.000000816	(15.2)
32	0.0144	(,	0.0000743	(0.0000000722	· <i>·</i> - <i>i</i>	0.0000000536	
	Wo	orst erro	r of grid	points a	and 0.01, 0.0	2,, 0	.99, 1.00.	
<u>n</u>	₩c <u>*</u>	orst erro	r of grid <u>0</u>	points a	and 0.01, 0.0 <u>1</u>	2,, 0	.99, 1.00. <u>2</u>	
<u>n</u> 2	Wc <u>*</u> 0.211	orst erro	r of grid <u>0</u> 0.0103	points a	and 0.01, 0.0 <u>1</u> 0.000404	(5,3)	.99, 1.00. <u>2</u> 0.000274	(13.6)
<u>n</u> 2 4	Wc <u>*</u> 0.211 0.113	(1.9)	r of grid <u>0</u> 0.0103 0.00369	<pre>points a (2.8) (3.4)</pre>	and 0.01, 0.0 <u>1</u> 0.000404 0.0000765	2,, 0 (5.3) (9.5)	.99, 1.00. <u>2</u> 0.000274 0.0000194	(13.6)
<u>n</u> 2 4 8	Wc <u>*</u> 0.211 0.113 0.0572	(1.9) (2.0)	r of grid <u>0</u> 0.0103 0.00369 0.00107	<pre>points a (2.8) (3.4) (3.7)</pre>	and 0.01, 0.0 <u>1</u> 0.000404 0.0000765 0.00000795	2,, 0 (5.3) (9.5) (8.9)	.99, 1.00. <u>2</u> 0.000274 0.0000194 0.00000128	(13.6) (15.1) (15.7)
<u>n</u> 2 4 8 16	Wc <u>*</u> 0.211 0.113 0.0572 0.0287	(1.9) (2.0) (2.0) (2.0)	r of grid <u>0</u> 0.0103 0.00369 0.00107 0.000288	points a (2.8) (3.4) (3.7) (3.9)	and 0.01, 0.0 <u>1</u> 0.000404 0.0000765 0.00000795 0.000000894	2,, 0 (5.3) (9.5) (8.9) (8.4)	.99, 1.00. <u>2</u> 0.000274 0.0000194 0.00000128 0.000000816	<pre>(13.6) (15.1) (15.7) (15.2)</pre>

TABLE 3. Example 3: $x(s) - \int_{0}^{s} \sin(s)\cos(t)x(t)dt = \sin(s) + (1-\sin(s))\exp(\sin(s))$. $x(s) = \exp[\sin(s)]$. Example 3 is the problem

$$x(s) - \int_{0}^{s} \sin(s) \cos(t) x(t) dt = \sin(s) + (1 - \sin(s)) e^{\sin(s)},$$

and the solution is $x(s) = \exp[\sin(s)]$. The results are very similiar to those of examples 1 and 2. An unexpected result is fourth order convergence on the grid points for r = 1. Notice that this occurred in example 2 also. We originally expected the convergence factors to be 2, 4, 8, 16 for r = *, 0, 1, 2 respectively. No adequate explanation has been presented as to why this phenomenon occurs.

Example 4 is the problem

$$x(s) - \int_{0}^{s} \sin(\pi st) x(t) dt = \begin{cases} s + \frac{\cos(\pi s^{2})}{\pi} - \frac{\sin(\pi s^{2})}{\pi^{2} s^{2}}, & 0 \le s \le \frac{1}{\pi} \\ \frac{(1-s)}{\pi s(\pi-1)} (1 + \cos(\pi s^{2})) \\ - \frac{\sin(s) - \frac{1}{\pi} \sin(\pi s^{2})}{(\pi-1)\pi s^{2}}, & \frac{1}{\pi} < s \le 1 \end{cases}$$
with solution $x(s) = \begin{cases} s, & 0 \le s \le \frac{1}{\pi} \\ \frac{1-s}{\pi-1} & \frac{1}{\pi} \le s \le 1, \end{cases}$

which was chosen to test the results of II.8. Note that the orderly convergence patterns are disrupted and we are no longer quite so sure convergence is occurring. But recall that no convergence rate was predicted for this case, simply that convergence would occur.

n	*		<u>0</u>		<u>1</u>	
2	0.0234	<i></i>	0.00321	<i></i>	0.000720	(. 1)
4	0.0166	(1.4)	0.000683	(4.5)	0.000670	(≈ ⊥)
8	0.00860	(1.9)	0.000771	(< 1)	0.000714	(~ 1)
16	0.00406	(2.0)	0.0000761	(3,3)	0.0000744	(3.3)
32	0.00203	(2.0)	0.0000230	(5.2)	0.0000227	
64	0.00102	(2.0)	0.00000441	(5.2)	0.00000307	(/•4)

Worst error of Grid Points

and 0.01, 0.02, ..., 0.99, 1.00.

<u>n</u>	*		<u>0</u>		<u>1</u>	
2	0.0234	(7 4)	0.00321	(4 0)	0.000870	(1 2)
4	0.0166	(1.4)	0.000683	(4.8)	0.000676	$(1 \cdot 3)$
8	0.00860	(1, 3)	0.000777	((10,0))	0.000716	(9.6)
16	0.00406	(2.0)	0.0000761	(3.3)	0.0000744	(3.8)
32	0.00203	(2,0)	0.0000230	(5,2)	0.0000227	(7.4)
64	0.00102	()	0.00000441	()	0.0000307	

TABLE 4. Example 4: $x(s) - \int_{0}^{s} \sin(\pi st) x(t) dt = f(s)$ where $x(s) = \begin{cases} s, & 0 \le s \le \frac{1}{\pi} \\ & \text{is a continuous function.} \\ \frac{1-s}{\pi-1}, & \frac{1}{\pi} < s \le 1, \end{cases}$ III. Applications to Fredholm Equations

III.1 Fredholm Equations with Jump Discontinuities

An easy extension of II.1 applies to Fredholm integral equations of the type

$$\mathbf{x}(s) - \int_{0}^{1} \mathbf{N}(s,t) \mathbf{x}(t) dt = f(s)$$

where

$$N(s,t) = \begin{cases} K(s,t), & 0 \le t \le s, \\ \\ R(s,t), & s < t \le l, \end{cases}$$

and where both K and R are continuous on their <u>closed</u> triangles of definition. That is, along the line s = tthere is a jump discontinuity in N with magnitude K(s,s) - R(s,s).

If in addition we assume that the rth partial derivatives with respect to t of K and R are at least piecewise continuous on their closed domains, then we can define a jump function

$$J^{(\ell)}(s) \equiv \frac{\partial^{\ell}}{\partial t^{\ell}} [K(s,t) - R(s,t)]_{t=s},$$

and proceed as in II.1:

$$f(s) = x(s) - \int_{0}^{1} N_{r}(s,t) x(t) dt$$
$$- \sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} J^{(\ell)}(s) \int_{0}^{s} (s-t)^{\ell} x(t) dt, \qquad (3-1)$$

where

$$N_{r}(s,t) = \begin{cases} K(s,t) - \sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} (s-t)^{\ell} J^{(\ell)}(s), & 0 \le t \le s \\ R(s,t), & s < t \le 1 \end{cases}$$

is a continuous kernel and has r continuous derivatives across the line s = t. Since both integrals in (3-1) can be well approximated by finite sums, it is reasonable to expect that the corresponding approximations, x_n , to the solution, x, will also be good. If r is large enough we would also expect fourth order convergence using repeated Simpson's rule and its modification.

III.2 An Example

The one-dimensional Green's function

$$G(s,t) = \begin{cases} t(1-s), & 0 \le t \le s \\ s(1-t), & s < t \le 1 \end{cases}$$

arises in two-point boundary value problems. As seen, G(s,t) is continuous, but its first derivative has a jump discontinuity along the line s = t. The problem

x(s) - 10
$$\int_{0}^{1} G(s,t)x(t) dt = (1 - \frac{10}{\pi^{2}}) \sin(\pi s)$$

was solved by first using the regular Simpson's rule approximation of the integral and then using the special rule. Since $J^{(l)}(s) \equiv 0$ for l = 0, and $l \geq 2$, r was chosen to be 1. The data are presented in table 5. Note that as predicted in II.7 there is fourth order convergence using the special rule, which is a significant improvement over the first order convergence of the regular Simpson's rule.

The worst error at the Grid Points

n	Regular	Special with $r = 1$
2	0.869	0.735
4	(1.5) 0.582	0.0303
8	0.252	0.00189
16	0.0770	0.000119

TABLE 5. The worst error at the partition points of the problem

$$x(s) - \int_{0}^{1} G(s,t) x(t) dt = (1 - \frac{10}{\pi^{2}}) \sin(\pi s),$$
$$x(s) = \sin(\pi s).$$

III.3 Generalizations

A generalization of the problem in III.l is one in which the discontinuity in N is along a continuous curve, g(s), $0 \le s \le 1$. The procedure is nearly the same, except that

$$J^{(\ell)}(s) \equiv \frac{\partial^{\ell}}{\partial t^{\ell}} [K(s,t) - R(s,t)]_{t=g(s)}$$

and

$$N_{r}(s,t) \equiv \begin{cases} K(s,t) - \sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} [g(s)-t]^{\ell} J^{(\ell)}(s), & 0 \le t \le g(s), \\ R(s,t), & g(s) < t \le 1. \end{cases}$$

The equation corresponding to (2-2) is

$$f(s) = x(s) - \int_{0}^{1} N_{r}(s,t) x(t) dt$$
$$- \sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} J^{(\ell)}(s) \int_{0}^{g(s)} [g(s)-t]^{\ell} x(t) dt$$

Note that now the upper limit of integration is a function of s, so that the special rule developed in II.2 will no longer work (unless $g(s) \equiv s$ of course). It should be relatively straight forward, however, to develop weights that are functions of both ℓ and g(s), using the same technique in II.2.

IV. Summary and Conclusions

We started with the Volterra integral equation (1-3)and generated a Fredholm integral equation with a continuous kernel. This was done by subtracting from K(s,t) the value of the discontinuity at s = t, namely K(s,s), leaving a Fredholm kernel which is zero for $s \le t \le 1$. The Fredholm kernel was made smoother across the line s = t by subtracting terms of Taylor's series; the resulting kernel was

$$N_{r}(s,t) = \begin{cases} K(s,t) - \sum_{\ell=0}^{r} \frac{(-1)^{\ell}}{\ell!} (s-t)^{\ell} K^{(\ell)}(s,s), & 0 \le t \le s \\ 0, & s < t \le 1. \end{cases}$$

Assuming that K and x have r continuous partials with respect to t, we showed that $\int_0^1 N_r(s,t)x(t)dt$ was well approximated by existing integration rules.

In order to preserve equality, terms of the form

$$\frac{(-1)^{\ell}}{\ell!} K^{(\ell)}(\mathbf{s},\mathbf{s}) \int_{0}^{\mathbf{s}} (\mathbf{s}-\mathbf{t})^{\ell} \mathbf{x}(\mathbf{t}) d\mathbf{t}$$

were added. In II.2 we developed a generalization of Simpson's rule which approximated the indefinite integral. In II.5 we combined this new rule with the regular Simpson's rule, and showed in II.7 that the resulting approximation has fourth order convergence assuming enough differentiability of the integrand. We also showed in II.8 that without differentiability the approximation still converges uniformly to the integral as $n \rightarrow \infty$. The work of II.5 developed an algorithm for solving linear Volterra integral equations of the second kind.

In the last chapter we extended the results to Fredholm integral equations with jump discontinuities in the kernel or one of its partial derivatives with respect to t along the line s = t.

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APPENDICES

Appendix A

begin comment a program to estimate $|R[x(s)]| \le (M_3/2) h^{\ell+4} \int_0^s |K[G_2(s-u)]| du$ where the h has been parameterized out of the integral. The integral is approximated by the repeated midpoint rule; integer n,tn,i,j,l; real s,t,rem,prod; real procedure Gn(a,b); value a,b; integer a; real b; Gn:= if b>0 then $b\uparrow a$ else 0.0; real procedure WB(b,c); value b,c; real b; integer c; $WB:=b^{(c+2)} \times ((2-b)/(c+1) + (2\times b)-2)/(c+2)-b/(c+3));$ real procedure WC(b,c); value b,c; real b; integer c; $WC:=-0.5 \times b^{+}(c+2) \times ((1-b)/(c+1) + (2\times b-1)/(c+2)-b/(c+3));$ comment the program body appears below; inreal (60,n); inreal (60, l); comment a statement to print n and l and set up a table for the output would occur here; $tn:=2 \times n;$ $prod:=(l+1) \times (l+2) \times (l+3);$ for j:=0 step 1 until tn do begin real temb, temc; s:=j/n;temb:=WB(s, l);

```
temc:=WC(s,l);
rem:=0.0;
for i:=l step l until tn do
    begin
    t:=(2×i-1)/tn;
    rem:=rem + abs(2×Gn(l+3,s-t)/prod
        -temc × Gn(2,2-t) - temb × Gn(2,1-t));
    end;
rem:=rem/n;
comment a statement to output s and the remainder,
        rem, at s would go here;
end;
```

end of program;

Appendix B

begin comment a program to solve a Volterra integral equation of the second kind using a modified Simpson's rule. integer n,r,tn,i,l,fac,j,P; real s,h,th,hsq,D,sn,hpw,tl,t,xs; real array X,F[0:UL]; comment UL is the upper limit of the array, i.e., UL $\geq 2 \times n$; comment the three weight functions are below. s=a, l=b, h=c and hsq = e;real procedure WA(a,b,c,e); value a,b,c,e; real a,c,e; integer b; $WA:=a^{(b+1)} \times (a \times (2.0 \times a - 3.0 \times c \times (b+3)) + 2.0 \times e \times (b+2)$ \times (b+3))/(2.0×e×(b+1) × (b+2) × (b+3)); real procedure WB(a,b,c,e); value a,b,c,e; real a,c,e; integer b; $WB:=2.0 \times a^{(b+2)} \times (c^{(b+3)}-a)/(e^{(b+1)} \times (b+2) \times (b+3));$ real procedure WC(a,b,c,e); value a,b,c,e; real a,c,e; integer b; WC:=a $(b+2) \times (2.0 \times a - c \times (b+3)) / (2.0 \times e \times (b+1) \times (b+2) \times (b+3));$ real procedure KER(a,b); value a,b; real a,b; comment evaluates the kernel K(s,t) at s=a and t=b; KER:=[the kernel];

```
real procedure PK(a,b);
value a,b;
integer b;
real a;
comment evaluate the bth partial of K(s,t) with respect to
        t at s=t=a;
    begin
    switch Q:=P0,P1,P2;
    real RL;
   <u>go to Q[b+1];</u>
P0: RL:=[the zeroth partial];
    go to fin;
Pl: RL:=[the first partial];
    go to fin;
P2: RL:=[the second partial];
fin: PK:=RL;
    end;
real procedure NR(a,b,c);
value a,b,c;
real a,b;
integer c;
comment evaluates the kernel Nr at s=a, t=b, and r=c;
    begin integer LL;
    real temp, nn,ff,dd,pp;
    if b>a then
        begin temp:=0.0; go to BBB end;
    temp:=KER(a,b);
    nn:=-1.0;
    dd:=a-b;
    for LL:=0 step 1 until c do
        begin
        ff:= if LL=0 then 1.0 else ff×LL;
        nn:=-nn;
```

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```
pp:= if LL=0 then 1.0 else dd × pp;
        temp := temp - nn × pp × PK(a,LL)/ff;
        end;
BBB: NR:=temp;
    end of procedure Nr;
real procedure FUN(a);
value a;
real a;
comment evaluates the known function at s=a;
FUN:=[the known function];
comment the program begins here. n is the number of
        times the rule is applied and r is the number
        of derivatives to be subtracted;
        eof (finished);
inreal (60,n);
inreal (60,r);
tn:=2 \times n;
for i:=0 step 1 until tn do
    begin
    s:=i/tn;
    F[i]:=FUN(s);
    end;
X[0] := F[0];
h:=1.0/tn;
th:=2.0 \times h;
hsq:=1.0/(tn \times tn);
D:=-h \times KER(h, 0.0)/3.0;
sn:=-1.0;
hpw:=1.0;
for l:=0 step 1 until r do
    begin
    fac:= if l=0 then 1 else fac × l;
    sn:=-sn;
    hpw:=h \times hpw;
```

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```
D:=D + sn \times PK(h, \ell) \times (hpw/3.0 - WA(h, \ell, h, hsq))/fac;
    end;
f[1]:=f[1] - D \times X[0];
for i:=2 step 1 until tn do
    begin
    s:=i/tn;
    F[i] := F[i] + h \times KER(s, 0.0) \times X[0]/3.0;
    end;
for j:=0 step 1 until n-1 do
    begin
    real temp,D1,D2,D3,D4,DET;
    integer p,q;
    p:=2 × j + 1;
    q:=p + 1;
    s:=p/tn;
    Dl:= if r < 0 then 1.0 - 4.0 × h × KER(s,s)/3.0
          else 1.0;
    sn:=-1.0;
for l:=0 step 1 until r do
    begin
    fac:= if l=0 then l else fac × l;
    sn:=-sn;
    Dl:=Dl - sn \times PK(s, \ell) \times WB(h, \ell, h, hsq)/fac;
    end;
D2:=0.0;
sn:=-1.0;
for l:=0 step 1 until r do
    begin
    fac:= if l=0 then 1 else fac \times l;
    sn:=-sn;
    D2:=D2 - sn \times PK(s, \ell) \times WC(h, \ell, h, hsq)/fac;
    end;
s:=q/tn;
t:=p/tn;
```

```
D3:=-4.0 \times h \times KER(s,t)/3.0;
D4:=1.0 - h \times KER(s,s)/3.0;
DET:=D1 \times D4 - D2 \times D3;
\underline{\text{if}} \text{ abs(DET)} < 10^{-7} \underline{\text{then}}
     begin
     comment a statement here would print "The problem
               generated a singular matrix.";
     go to finished;
     end;
X[p] := (F[p] \times D4 - F[q] \times D2) / DET;
X[q] := (F[q] \times D1 - F[p] \times D3) / DET;
if j = n-1 then go to otpt;
s:=(q+1)/tn;
temp:=4.0 \times h \times KER(s,t)/3.0;
t:=q/tn;
D:=2.0 \times h \times KER(s,t)/3.0;
sn:=-1.0;
hpw:=1.0;
for l:=0 step 1 until r do
     begin
     fac:= if l=0 then 1 else fac × l;
     sn:=-sn;
     hpw:=h × hpw;
     D:=D - sn \times PK(s, l) \times (hpw/3.0-WA(h, l, h, hsq))/fac;
     end;
F[q+1]:=F[q+1] + temp \times X[p] + D \times X[q];
tl:=p/tn;
for i:=q+2 step 1 until tn do
     begin
     s:=i/tn;
     F[i]:=F[i] + 4.0 \times h \times KER(s,t1) \times X[p]/3.0 + 2.0 \times h
             \times KER(s,t) \times X[q]/3.0;
     end;
```

end;

```
comment a statement to print the problem, the
otpt:
                values of n and r, and column headings
                would go here;
        for i:=0 step 1 until tn do
            begin
            s:=i/tn;
            comment a statement to output s and
                     X[i] = x(s) would go here;
            end;
comment the interpolation begins here. Values of s
                                                             are
         input until there are no more, whereupon the
         eof (finished) command halts the program;
    begin real xs,tl,t2,t3; integer Il;
inter: comment a statement goes here to input s;
    if s=0.0 then begin j:=0; go to AAA end;
    for i:=0 step 1 until n-1 do
    if 2 \times i \times h < s \wedge (2 \times i + 2) \times h > s then
         begin j:=i; go to AAA end;
AAA:
      xs:=FUN(s);
      for i:=0 step 1 until j-1 do
         begin
         Il:=2 × i;
         tl:=Il × h;
         t2:=(I1+1) \times h;
         t3:=(I1+2) \times h;
         xs:=xs + (KER(s,t1) \times X[I1] + 4.0 \times KER(s,t2) \times X[I1+1]
             +KER(s,t3) ×X[I1+2]) × h/3.0;
         end;
II:=2 \times j; tI:=II \times h; t2:=(II+1) \times h;
xs:=xs + (NR(s,tl,r) \times X[I1]+4.0 \times NR(s,t2,r) \times X[I1+1]) \times h/3.0;
sn:=-1.0;
tl:=s - 2.0 \times h \times j;
for i:=0 step 1 until r do
    begin
```

```
fac:= if i=0 then l else fac × i;
sn:=-sn;
xs:=xs + sn × PK(s,i) × (WA(tl,i,h,hsq)×X[Il]
+WB(tl,i,h,hsq)×X[Il+1]+WC(tl,i,h,hsq)
×X[Il+2])/fac;
```

end;

comment a statement here would output s and xs = x(s); end;

finished: end of program;