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AN EFFICIENT NUMERICAL SOLUTION OF SECOND-KIND FREDHOLM INTEGRAL EQUATIONS USING THE NYSTRÖM METHOD WITH ADAPTIVE QUADRATURE RULES

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Abstract
An efficient adaptive Nyström method for the solution of linear Fredholm integral equations of the second kind is presented. The method does not place quadrature nodes uniformly throughout the length of the integration interval, but rather estimates the local error of the quadrature in each subinterval and refines only those subintervals which contribute most to the overall error. A composite Gauss–Legendre pair is used to produce coarse and refined approximations; other composite methods, such as adaptive Simpson or composite Gauss–Kronrod can be applied as well. Next, the quadrature nodes and weights are used to form the Nyström linear system, which is modified as the mesh is refined. The method is based on local error estimates, global tolerance control, condition-number checks, algebraic residual testing and solution-error estimation on a dense grid, to ensure accuracy and numerical stability. The primary advantage is that the relatively few quadrature points are concentrated in regions of the kernel/solution where it is rapidly varying or less smooth, and the relatively large subintervals can be used over more smooth regions. From this error analysis, it is seen that the overall numerical error is related to the quadrature approximation as well as the amplification caused by the inverse of the discrete Fredholm operator. A reliable stopping criterion should take into account the estimated quadrature error as well as the residual of the linear system, for this reason. Computational complexity, implementation procedures, convergence conditions and reproducibility of the paper are also discussed. In general, the adaptive approach is particularly helpful in problems involving localized variations, boundary layers, oscillatory behaviour or pieces that are not necessarily smooth, where uniform quadrature rules could be overly expensive in terms of number of function evaluations.

1. Introduction
Second kind Fredholm integral equations are found in boundary integral equations, potential theory, elasticity, radiative transfer, electromagnetic scattering and models with nonlocal interactions. The identity-plus-integral structure is, in general, more stable than a first-kind formulation, but an analytic solution is seldom available for realistic kernels (Atkinson, 1997; Baker, 1977; Delves & Mohamed, 1985; Jerri, 1985; Kress, 2014).The standard linear equation is

$$f(x) - \lambda \int_a^b K(x,t)f(t)dt = g(x), \quad a \leq x \leq b. \quad (1)$$

The Nyström method can approximate the integral, and requires the resulting equation to be satisfied at the quadrature nodes. In this manner, Equation (1) can be solved as a finite system of linear equations, with the solution being reconstructed continuously over the interval (Nyström, 1930; Atkinson, 1974; Occorsio & Russo, 2014). The commonly used methods are the fixed quadrature rules, including the midpoint, trapezoidal, Simpson's, and Gauss–Legendre rule (Burden et al., 2016; Davis & Rabinowitz, 1984). If the integrand is sufficiently smooth throughout [a,b] (mildly like the uniform grid), then a uniform grid is generally good. When the integrand is not smooth over the whole interval, or oscillates or changes rapidly, however, only in a small part of it, the computational effort can be spent evenly even if the integrand is not smooth in that part—then the algorithm is not efficient.

The adaptive quadrature overcomes this restriction by estimating the error in each subinterval and only refining panels where a higher accuracy is required. The standard adaptive integration methods employ nested and paired quadrature rules, priority-based panel selection and systematic tolerance allocation, and require a minimum number of function calls for a desired accuracy (Piessens et al., 1983; Press et al., 2007). When using Nyström for numerical solution, however, particular attention must be given to the ideas because the quadrature nodes are also collocation points, and thus have direct impact on the size and conditioning of the linear system that is solved.

The objective of this paper is to create an efficient adaptive Nyström method, to set up a practical error-control strategy, to give a repeatable implementation procedure, and to analyze the computational advantages/disadvantages of the method. The proposed approach is to employ a common panel partition which is adaptively refined throughout the entire kernel. This will make the same set of nodes used to build the discrete integral operator during the entire calculation.

2. Nyström discretization

Let T be the integral operator

$(Tf)(x) = \int_a^b K(x,t)f(t)dt.$ (2)

A quadrature formula with nodes t_j and weights w_j gives

$(T_m f)(x) = \sum_{j=1}^{m} w_j K(x,t_j) f(t_j).$ (3)

The Nyström approximation at an arbitrary point is

$f_m(x) = g(x) + \lambda \sum_{j=1}^{m} w_j K(x,t_j) f_j.$ (4)

Collocation at $x=t_i$ produces

$\sum_{j=1}^{m} [\delta_{ij} - \lambda w_j K(t_i,t_j)] f_j = g(t_i), \quad i = 1,\dots,m.$ (5)

With $K_m=[K(t_i,t_j)]$, $W=\mathrm{diag}(w_1,\dots,w_m)$, and $A_m=I-\lambda K_m W$, the discrete system is

$A_m f = g_m.$ (6)

The weight w_j scales column j since it is part of the integration variable t_j. In general the matrix is dense. The number of kernel evaluations needed for assembly is $O(m^2)$, storage is $O(m^2)$ and the factorization procedure directly costs $O(m^3)$ operations (Golub & Van Loan, 2013). Therefore, an effective adaptive strategy has to decrease the number of nodes without compromising the stability.

3. Adaptive quadrature framework

3.1 Panel-based quadrature

Divide [a, b] into panels P_r of $[\alpha_r, \beta_r]$. Apply a p-point Gauss–Legendre rule Q_r^p on each panel, and a refined rule by bisecting the panel and applying the same rule to each segment. The refined approximation is called Q_r^{2p}. The quadrature points used on each panel are mapped from the interval $[-1,1]$ and the global quadrature is simply the sum of the quadratures over all the panels (Gautschi, 2004; Golub & Welsch, 1969).

$Q^A(q)=\sum_r Q_r^p(q).$ (7)

A Gauss–Kronrod pair may be used to save the value of the function, and the adaptive Simpson is convenient on uniform nested points. The paired-Gauss form is used here because it is exactly polynomial locally and is easily subdivided into panels.

3.2 Local defect estimator

For a current Nyström approximation $\tilde{f}$ and a representative collocation or monitoring point x_i,

define $q_i(t)=K(x_i,t)\tilde{f}(t)$. The local defect on panel P_r is estimated by

$$\eta_{ir} = |Q_r^{2p}(q_i) - Q_r^{p}(q_i)|. \quad (8)$$

Because a single panel mesh must serve every x, the panel indicator combines several monitoring points:

$$\eta_r = max_i \in M\ \eta_{ir}. \quad (9)$$

The monitoring set M contains the current collocation nodes and may include endpoints or additional check points. A maximum indicator is conservative; a weighted root-mean-square indicator may be used when the problem is large. Panel P_r is marked when

$$\eta_r > \tau_r, \quad \tau_r = \tau abs(\beta_r - \alpha_r)/(b-a) + \tau rel\, S_r. \quad (10)$$

Here τabs and τrel are requested absolute and relative tolerances, and S_r is a local scale such as $\max_i |Q_r^{2p}(q_i)|$. Length-weighted allocation prevents a large number of short panels from each receiving the full global tolerance. Error-controlled Nyström strategies similarly require the quadrature defect to be connected to the solution process rather than treated as an unrelated integration calculation (Dobner, 1994).

3.3 Adaptive refinement cycle

1. A nonlinear looking refinement loop has no effect on the underlying linear equation. Changes only the discrete operator and solves the linear system. The procedure is:
2. Set up a coarse partition of the panel and select a local quadrature order p.
3. 2. Create all the mapped nodes and weights; group together duplicate boundary nodes if endpoints are selected in the rule.
4. 3. Construct A_m, g_m, estimate cond(A_m), and solve the equation $A_m\tilde{f}=g_m$ using a stable factorization.
5. At the refined-rule nodes, evaluate $\tilde{f}$ by extending it with the Nyström extension in Equation (4).
6. Calculate η_r for each panel using Equations 8-10.
7. Divide marked panels; retain unmarked panels and quadrature data.

Repeat assembly, solution and estimation until global defect, algebraic residual and solution–change tests are satisfied or until a resource limit is reached.

4. Efficient numerical implementation

4.1 Data structures and reuse

Each panel has endpoints, quadrature nodes and weights, local error indicator, and current refinement level stored. If nodes are not changed, then the corresponding kernel matrix blocks can be stored and reused; however, the dense matrix will need to be extended whenever new quadrature nodes are added.

If the system is not very large, it is frequently the easiest and most reliable solution to re-compute the entire matrix at every refinement. In larger problems, the cost can be lowered by running blockwise updates, by using iterative linear solvers or by using low rank approximations to the kernel matrix (Gittens & Mahoney, 2016; Williams & Seeger, 2001).

4.2 Stopping criteria

None of the indicators on their own is enough. The algorithm only terminates when all three conditions are true:

$$\eta global = \sum_r \eta_r \le \tau abs + \tau rel\|\tilde{f}\|_\infty, \quad (11)$$

$$Rrel = \|g_m - A_m\tilde{f}\|_\infty / \max(1,\|g_m\|_\infty) \le \tau lin, \quad (12)$$

$$\Delta rel = \|\tilde{f}new - \tilde{f}old\|_{G,\infty} / \max(1,\|\tilde{f}new\|_{G,\infty}) \le \tau sol. \quad (13)$$

The successive adaptive meshes have different nodes, thus the last norm is tested on a fixed independent grid G. The residual tests for accuracy of the algebraic solve, the solution-change test tests for mesh convergence, and ηglobal is the remaining quadrature defect. You can use maximum refinement level and maximum node count to stop the subdivision from going too far.

4.3 Complexity

If the final adaptive mesh contains m_a nodes and a comparable uniform mesh requires m_u nodes, the direct-solve cost ratio is approximately $(m_a/m_u)^3$. Even a moderate reduction in node count can therefore yield a substantial gain. Adaptive refinement has overhead from error estimation and repeated solves, so it is most valuable when difficulty is localized. For globally smooth analytic data, one sufficiently high-order

Gaussian rule may be faster than repeated adaptation. For globally oscillatory data, many panels may be refined and the advantage may diminish.

Table 1. Computational comparison of fixed and adaptive Nyström discretizations.

Component	Fixed quadrature	Adaptive quadrature	Efficiency consideration
Node distribution	Predetermined, often uniform	Concentrated on marked panels	Adaptive nodes reduce waste in smooth regions
Error information	Usually obtained after mesh refinement	Local indicator available every cycle	Supports automatic stopping
Linear solves	One per selected mesh	Several as the mesh evolves	Warm starts or block updates may help
Kernel evaluations	$O(m_u^2)$	$O(m_a^2)$ plus estimator evaluations	Beneficial when m_a is substantially smaller
Best use	Uniformly smooth data	Localized variation or weak regularity	Problem structure determines advantage

5. Error and convergence analysis

Let T_m^A be the adaptive quadrature operator. Subtracting the continuous and discrete equations gives

$$(I - \lambda T_m^A)(f - f_m) = \lambda(T - T_m^A)f. \quad (14)$$

If the discrete inverse exists,

$$\|f - f_m\|\infty \leq |\lambda|\|(I - \lambda T_m^A)^{-1}\|\infty \|(T - T_m^A)f\|\infty. \quad (15)$$

Equation (15) shows that the adaptive quadrature estimator controls only the consistency term. The final solution error is amplified by the discrete resolvent. When λ is close to a characteristic value, A_m may be ill-conditioned and a small local quadrature defect may not produce a small solution error (Atkinson, 1997; Kress, 2014). Condition estimation is therefore an essential part of adaptive error control.

For sufficiently smooth panel integrands, increasing p yields high-order local convergence. When smoothness is nonuniform, h-refinement reduces the panel length near difficult regions. A combined hp strategy can raise p on smooth panels and bisect panels where convergence with p stagnates. Typically, a weak singularity needs to be subtracted, integrated via a product or transformed using a coordinate change (Brunner, 2004).

If a precise solution exists, the accuracy should be determined independently,

$$E_{dense} = \max_{x \in G} |f(x) - \tilde{f}_m(x)|. \quad (16)$$

Efficiency is measured by plotting the Edense algorithm on the following: kernel evaluations, number of nodes, elapsed time, and peak memory. Error comparisons are inaccurate if they are made only with the number of refinement cycles, as there are many different types of cycles and they can add different numbers of nodes.

6. Numerical test design

A performance study should be reproducible, and must include manufactured solutions. Define the functions f and K:

$$g(x) = f(x) - \lambda \int_a^b K(x,t)f(t)dt. \quad (17)$$

The tested method must have a higher accuracy than the analytical evaluation of the integral defining g. Three complementary tests are recommended: Smooth analytic kernel, Localized layer kernel/solution, Oscillatory kernel. The smooth test starts to define high-order behavior, the localized test is used to measure the value of the adaptation, and the oscillatory test is used to see if the indicator is responsive to repeated hard-to-do regions.

Table 2. Recommended numerical tests for adaptive Nyström performance.

Test class	Representative structure	Expected adaptive response	Reported measures
Smooth analytic	$K(x,t)=e^{xt}$ with smooth f	Few large panels; high-order rule dominates	Edense, nodes, time, $\kappa(A)$
Localized layer	K or f changes rapidly near $t=t_0$	Strong refinement near t_0; coarse elsewhere	Panel map, Edense, evaluations
Oscillatory	$K(x,t)=\cos(\omega xt)$ for moderate or large ω	Multiple refined panels as ω grows	Error versus ω and node count
Near-sensitive operator	λ chosen near a characteristic value	Conditioning may dominate quadrature error	$\kappa(A)$, residual, estimator reliability

For all experiments, the following quantities should be reported: τabs, τrel, τlin, τsol, p, initial mesh, max refinement level, arithmetic accuracy, and linear solver. Fixed rule comparisons must be based on the same equation and accuracy goal. It is not necessarily a measure of good performance that it takes the same number of subdivisions for a method to achieve that target, but rather of how much effort is needed to reach that target.

7. Discussion

The adaptive quadrature allows the Nyström method to be made into an error-controlled computation method. The main benefit of it is selective refinement which is the subdivision of panels based on the behaviour of the resulting product of the kernel and the solution, rather than on a uniform pattern. This can significantly decrease the number of quadrature nodes. Thus, even if the number of nodes is not so large, then the number of reduced nodes can cause a significant reduction in the cost of matrix factorization for the Nyström method, because the resulting matrix is dense.

There are, however, a number of practical issues to consider with adaptivity. The local error estimator should be based on sufficiently many (x)-values to reflect the behavior of the integral operator, the successive numerical solutions should be compared at a common grid, and the conditioning of the discretized system needs to be checked during the refinement procedure. Only refining the mesh using a single value of (x) might not capture all the features of the kernel, which could be important at other values of (x). Evaluation of all local error indicators at all collocation points, on the other hand, could be expensive. A reasonable compromise is to use the collocation points in addition to a relatively small and fixed number of monitoring points, with a larger number of monitoring points as the reliability of the estimator is questioned. In the case of smooth periodic problems, a fixed trapezoidal rule might already converge very rapidly, and should thus be added as a benchmark rule (Trefethen & Weideman, 2014).

An advantage of using adaptive Simpson and Gauss–Kronrod rules is that the values of functions evaluated at the first half points are also used for the evaluation of the second half points, thereby avoiding the need to recompute the function values. Piessens et al. (1983) show that this reduces the cost of error estimation. By comparison, paired Gauss–Legendre rules give high order accuracy and are easily mapped onto each panel, but might need repeated evaluations. This is because the most suitable rule will be determined by the cost of assessing the kernel and how accurate the result needs to be. This proposed framework is not specific to a quadrature pair, but instead assumes that the nodes and weights from any pair can be used to form a single consistent global quadrature operator.

8. Conclusion

In this paper, an efficient Adaptive Nyström scheme is proposed for the solution of second kind Fredholm integral equation. The algorithm starts by building a common panel mesh and by solving the common weighted-kernel linear

system. It then calculates the local quadrature error by applying a pair of rules and adapts only those panels that need more resolution. It can be carried on until the quadrature-error estimates, algebraic residuals and changes in successive numerical solutions meet the required tolerances. The error analysis reveals that the consistency error caused by the numerical integration is controlled by adaptive quadrature and the inverse of the discrete operator controls the effect on the final solution. The technique is particularly useful for problems which have local variations in their solutions, boundary layers, limited regularity, or irregular oscillatory behavior. However, when the problem is uniformly smooth and analytic the fixed high-order quadrature rule can still be more efficient.

The implementation must be reliable, weights applied column-wise, a linear system solved with reliable numerical methods, and conditioning of the matrices checked during the refinement process. The accuracy should also be checked independently in another grid, and tolerances, nodes number, refinement number and residuals, computational effort should be reported clearly. These features, when combined, give an accurate, reliable and computationally efficient framework to solve many second kind Fredholm integral equations.

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