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QUADRATURE ERRORS IN FINITE ELEMENT EIGENVALUE COMPUTATIONS

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Abstract

Some recent results on the optimal choice of quadrature rules for the finite element solution of eigenvalue problems are discussed in the light of some results of the author and J. Paine.

Finite element solution of eigenvalue problems for differential equations leads to the matrix eigenvalue problem $A\mathbf{x} = \lambda B\mathbf{x}$, where the elements of the matrices A and B are integrals which are usually evaluated numerically. Quadrature errors in evaluating these integrals can significantly affect the accuracy of the computed solutions. This paper considers the implications of some earlier results of the author and J. Paine for some recent results on the optimal choice of quadrature rules for these problems.

The effect of quadrature errors on rather general variational methods was considered in [14]. That analysis explains why finite element methods, and indeed most variational methods in common use today, perform better than some classical variational methods, which used "nearly" linearly dependent coordinate functions. Some early results on the effect of quadrature errors in several finite element calculations are given in [12]. For eigenvalue problems involving self-adjoint second-order linear differential operators acting on functions defined on a polygonal domain in n-dimensional space, these results were significantly strengthened by Banerjee and Osborn [7]. They considered simplicial finite elements (line segments for $n = 1$, triangles for $n = 2$, *etc.*) of maximal diameter h. They established sufficient conditions for the finite element approximations, obtained when numerical quadrature is used, to be optimal in the sense that if, for some p, the error in the finite element approximation is $O(h^p)$ when there are no quadrature errors, then the error obtained when there are quadrature errors is also $O(h^p)$. Roughly, these conditions are that the eigenfunctions be sufficiently smooth and that the order of the quadrature rule used be sufficiently high. In particular they showed that, for sufficiently smooth eigenfunctions, if the error in the finite element eigenvalue approximations is $O(h^{2p})$ in the absence of quadrature errors,

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then these errors will still be $O(h^{2p})$ when numerical quadrature is used, provided the quadrature rule is exact for all polynomials of degree $2p-1$. Analogous results, with optimality criteria appropriate for the p-version of the finite element method, are proved in [8]. In [6], it is shown that the results of [7] are sharp for eigenvalues but not for eigenvectors. Stronger results for eigenvectors are proved in [6] and [13]. For two-dimensional problems, using rectangular piecewise linear finite elements, some results analogous to those of [7] are proved in [20] for non-polygonal regions. Some key results of [7] are extended in [19] to more general problems on composite structures, and some of these are further strengthened in [18].

A major limitation of the above results is that they are "optimal" only in the sense that they give the optimal power of h. Proving that the error is bounded above by an expression of the form Ch^p says nothing about the effect of quadrature errors on the coefficient C. Earlier results of the author and Paine [2, 5] show that quadrature errors can increase this coefficient (and hence the total error) considerably, so that it is still worthwhile to use more accurate quadrature schemes. In [5] we considered finite element solution of the Sturm-Liouville problem

$$-y'' + qy = \lambda y, \qquad y(0) = y(\pi) = 0,$$

using linear hat coordinate functions with a uniform mesh. The results of [7] show that, with this method, results obtained when the integrals are evaluated by the trapezoidal rule will be "optimal" in the sense that the "exact" finite element approximations to the eigenvalues have error $O(h^2)$ and the additional error introduced by this quadrature is also $O(h^2)$. However, results of [5] show that this numerical quadrature nevertheless significantly reduces accuracy.

It is well known that the error in the approximation to the kth eigenvalue of regular Sturm-Liouville problems obtained by the finite element method with linear hat coordinate functions and uniform mesh length h is $O(k^4h^2)$. In [5] we showed that the additional error introduced by the trapezoidal rule was $O(k^2h^2)$, this result being sharp. It might be thought that this would be subsumed in the larger $O(k^4h^2)$ error so that the trapezoidal rule would seem quite satisfactory. However, the main result of [5] is that the $O(k^4h^2)$ error of the finite element eigenvalues can be reduced, at negligible extra cost, to $O(k^2h^3/\sin(kh))$ — effectively $O(kh^2)$ for $kh < \pi/2$ — by a simple correction technique, first studied in connection with the classical second-order finite difference method in [15]. The idea is that, for both this finite difference method and the finite element method with linear hat coordinate functions, the error in the computed solution (in the absence of quadrature and round off errors) is known in closed form, in the special case of constant q, and that *this known error for constant q provides a good estimate of the error for sufficiently smooth nonconstant q*. This makes it easy to calculate a more accurate "corrected" solution. Following [1], we call this correction technique "asymptotic correction", as it is based on the different asymptotic behaviour of the eigenvalues of the differential equation and its discrete approximations. This name has been used in some other papers, but other names have also been used in the literature, including "algebraic correction" [9] and "the AAdHP correction" [16]. When this correction is used, the $O(k^2h^2)$ error produced by the use of the trapezoidal rule becomes the dominant error and a more accurate quadrature is clearly required. Moreover, numerical results in [5] with $q(x) = e^x$ show that, even without this correction, use of the trapezoidal rule more than doubles the error in the finite element approximation to the fundamental eigenvalue. Numerical results also showed that the corrected results are often considerably more accurate than shown by the theoretical bounds proved in [5], so that the effect of quadrature errors becomes even more important.

One way of dealing with these errors is to use a higher-order quadrature rule. It is shown in [5] that, if Simpson's rule is used, then the $O(k^2h^3/\sin(kh))$ accuracy of the corrected linear hat finite element estimates is preserved. Indeed it is shown in [3] that, subject to the same smoothness assumptions as were made in the proofs in [12], the additional error produced by using Simpson's rule instead of exact quadrature is $O(k^2h^4)$, as had been conjectured in [5] on the basis of numerical results. Perhaps a better strategy is to use product integration. There has been a great deal of research on the use of product integration to evaluate difficult integrals, some of it by Australian mathematicians [10, 11, 17], but very little attention appears to have been given to its potential use in the finite element method. Yet integrands arising in the finite element method are typically of the form qf, where q does not vary rapidly over the individual elements and f is a polynomial which varies rapidly but can be integrated in closed form. Product integration rules should be able to take advantage of this special product form of the integrand. This is discussed in more detail in [5] and [3]. Numerical results in [2, 3] using the product midpoint rule, and substantial unpublished numerical results of John Paine, support the usefulness of this approach.

Most papers on the effect of quadrature errors in finite element eigenvalue computations do not consider how the error grows with the order, k, of the eigenvalue. Presumably this is because, even with exact quadrature, the errors in the uncorrected finite element estimates grow rapidly with k, and it was thought that this was more important than the increase with k in the effect of quadrature errors. However, this argument is not valid if asymptotic correction proves as effective as for the problem studied in [5]. The theory of asymptotic correction has advanced considerably since the publication of [5]. Most of the theoretical results of [5] are extended to problems with natural or periodic boundary conditions in [2] and, as in [5], numerical results show that in practice the method often performs considerably better than has yet been proved. Numerical results (but not yet proofs) are also available which show that asymptotic correction can produce similar improvement to the results obtained by higher-order finite element methods. Still more accurate quadrature methods will be required to take advantage of this, and this may provide still stronger reasons for using some product integration scheme. A survey of results on asymptotic correction up to 1993 is given in [4] and there have been further developments since then, especially in its application to inverse eigenvalue problems [9].

Recent work on quadrature errors in finite element calculations has been mainly concerned with partial differential equations, which present a greater challenge than ordinary differential equations, and the theory is not restricted to uniform meshes. However, results proved so far for asymptotic correction almost all concern only ordinary differential equations with uniform mesh. Nevertheless numerical results in [1, 9] indicate that asymptotic correction can often be just as successful with partial differential equations. A major difficulty with extending asymptotic correction to partial differential equations is that there are not many problems with known closed form solution to be used for the correction. For this reason, [1] and [9] considered only the problem $-\nabla^2 u + qu = \lambda u$, with u vanishing on the boundary of a rectangle. Some difficulties arising with this particular problem are discussed in more detail in [9]. However, although more work is required before asymptotic correction can be used as easily with partial differential equations as it can now be used with Sturm-Liouville problems, any development with the potential for increasing the accuracy of finite element estimates obtained in the absence of quadrature errors provides an additional reason why it is worth increasing the accuracy of the numerical quadrature used in the process.

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