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Short note

Short note on the mass matrix for Gauss–Lobatto grid points

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ABSTRACT

The mass matrix for Gauss–Lobatto grid points is usually approximated by Gauss–Lobatto quadrature because this leads to a diagonal matrix that is easy to invert. The exact mass matrix and its inverse are full. We show that the exact mass matrix *and* its inverse differ from the approximate diagonal ones by a simple rank-1 update (outer product). They can thus be applied to an arbitrary vector in $O(N)$ operations instead of $O(N^2)$.

1. Motivation

With the increased emphasis on higher-order methods for solving partial differential equations, methods that divide the domain into subdomains and represent the solution as an expansion in basis functions have become more and more important. These include spectral element methods (penalty-based or continuous) and discontinuous Galerkin methods. To handle nonlinearities, collocation schemes are often the method of choice. In such methods, the expansion coefficients are replaced by function values at specially chosen grid points as the fundamental unknowns. In one dimension, the grid points are universally chosen to be the Gaussian quadrature points corresponding to the basis functions. This connects the expansion coefficients in spectral space to the function values in physical space by a discrete transform and leads to rapidly convergent and stable methods for smooth solutions.

In two and three dimensions, if the subdomains can be mapped to squares or cubes, then basis functions that are tensor products of one-dimensional basis functions are almost always used because of the resulting simplification of element-wise operations. Unless the problem requires the flexibility of grids constructed using triangles or tetrahedra, this approach is again almost universal. The key result of this note applies to any one-dimensional set of grid points that define a Gaussian quadrature or are part of a tensor product of such grid points. It does not apply to typical basis sets for triangles, where the quadrature rule and the choice of grid points are not directly connected.

For many problems, the simplest formulation uses Gauss–Lobatto collocation points since having grid points on the boundaries makes it easy to impose boundary conditions. In such a formulation, the exact mass matrix and its inverse are full. Thus it is natural to approximate the mass matrix by Gauss–Lobatto quadrature, which leads to a diagonal matrix that is easy to invert. By contrast, using Gauss collocation points with ordinary Gauss quadrature gives the exact mass matrix, which is diagonal. This makes the comparison between the two choices tricky. On the one hand, Gauss–Lobatto avoids interpolation from the interior points to the boundaries, but on the other hand it may require more collocation points

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to achieve the same accuracy as using Gauss points if you use the approximate mass matrix for efficiency. This point is discussed further in Section 4.3.

We show that there is a simple expression for the exact mass matrix and its inverse for Gauss–Lobatto collocation. Multiplying a vector by one of these expressions can be done in $O(N)$ operations, just as for a diagonal matrix. This suggests that efficiency versus accuracy results for implementations of spectral methods should be reconsidered. Of course, for large values of N the spectral convergence of Gaussian quadrature is likely to make the difference between the exact and approximate mass matrices irrelevant. However, for small or moderate N the situation is not clear.

2. Spectral approximation

This section summarizes some standard material [1–4] on spectral approximations in order to derive the key result in the next section.

Consider approximations of functions by expansions in orthogonal polynomials:

$$u(x) = \sum_{k=0}^{N} b_k p_k(x) \tag{1}$$

where

$$\int_{-1}^{1} p_j(x) p_k(x) W(x)\, dx = h_k \delta_{jk} \tag{2}$$

The associated inner product is

$$\langle u|v\rangle \equiv \int_{-1}^{1} u(x) v(x) W(x)\, dx \tag{3}$$

For simplicity, we will take the weight function $W(x) = 1$, in which case the basis functions are Legendre polynomials. However, almost everything in this note goes through for other systems of orthogonal polynomials.

The set of orthogonal polynomials determines a Gaussian quadrature formula with weights w_j and grid points x_j:

$$\int_{-1}^{1} f(x)\, dx \approx \sum_{j=0}^{N} w_j f(x_j) \tag{4}$$

The Gauss–Lobatto version of this quadrature arranges for the endpoints of the interval to be included in the set x_j. Having collocation points on the boundary can make the application of boundary conditions easier. The quadrature (4) is exact for polynomials of degree no more than $2N+1$ for the Gauss case and $2N-1$ for the Gauss–Lobatto case. Use the quadrature to define the discrete inner product as the analog of (3):

$$\langle u|v\rangle_{\mathrm{G}} = \sum_{j=0}^{N} w_j u(x_j) v(x_j) \tag{5}$$

The continuous and discrete inner products are the same if the product uv is a polynomial of degree no more than $2N+1$ (Gauss) or $2N-1$ (Gauss–Lobatto).

Eq. (1) is called a modal expansion. In collocation methods, instead of regarding the $N+1$ modal coefficients b_k as fundamental, we choose a set of $N+1$ collocation points x_j. Typically these are the Gauss or Gauss–Lobatto points associated with the orthogonal polynomials. The corresponding nodal expansion is

$$u(x) = \sum_{j=0}^{N} u_j \ell_j(x) \tag{6}$$

where $u_j \equiv u(x_j)$. The basis functions $\ell_j(x)$ are called cardinal functions and are simply the Lagrange interpolating polynomials based on the grid points x_j, with $\ell_j(x_i) = \delta_{ij}$:

$$\ell_j(x) = \prod_{\substack{i=0 \\ i\neq j}}^{N} \frac{x - x_i}{x_j - x_i} \tag{7}$$

The nodal expansion (6) is just an approximation of a continuous function $u(x)$ by its interpolating polynomial, so that $u(x_i) = u_i$. Note that in the discrete inner product (5) of any two continuous functions, we may replace u, say, by its