Gauss and Anti-Gauss Block Quadrature

D. Martin

Department of Mathematical Sciences, Kent State University

The present work is concerned with computing approximate bounds for elements of the quantity $W^T f(A)W$, where f is a smooth function, $W \in \mathbb{R}^{n\times k}$ has orthonormal columns, and $A \in \mathbb{R}^{n\times n}$ is a real symmetric matrix. The techniques generally used in the case $k = 1$ do not generalize to the case $k > 1$. In the scalar setting, Laurie introduces the $(n + 1)$-point anti-Gauss quadrature rule whose error is exactly opposite the error of the n-point Gauss rule for polynomials of degree at most $2n + 1$; together, the Gauss and anti-Gauss rules can be used to compute approximate bounds which hold when the Fourier coefficients of f decay sufficiently rapidly. We introduce the anti-Gauss quadrature rule for the block Lanczos algorithm, allowing computation of approximate bounds for elements of $W^T f(A)W$ when $k > 1$. We also discuss the nonsymmetric block Lanczos algorithm, and introduce the corresponding Gauss and anti-Gauss quadrature rules. This provides a means of computing approximate bounds for elements of $W^T f(A)V$ where $W, V \in \mathbb{R}^{n\times k}$ satisfy $W^T V = I_k$ and $A \in \mathbb{R}^{n\times n}$ is real but possibly not symmetric. Here, I_k is the $k \times k$ identity matrix. We discuss application to functions of a symmetric or nonsymmetric adjacency matrix, and numerical examples exhibit the validity of the bounds in this setting.