Gauss-Kronrod Quadrature

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1 Introduction

Our goal is to approximate

$$\int_a^b f(x)dx \tag{1}$$

numerically with adaptive integration. In other words, we want to use different grid sizes for different regions of the interval (a, b) depending on how quickly f changes there.

An adaptive quadrature scheme splits the interval into panels, approximates the integral on each panel using a quadrature rule, computes an estimate of the error of this rule on each panel, and if the error is too large, then that panel is further split into smaller panels and the process repeats. An important part of this process is computing an accurate error estimate of the quadrature rule on each panel. In practice, two quadrature rules (one higher order than the other) are applied to compute two different estimates of the integral and the error between them is used to estimate the error of the higher order quadrature rule.

Gauss-Kronrod quadrature does this cheaply by reusing the grid points of the lower order rule and adding new ones to create a higher-order rule, so that the number of function evaluations is equal to the number of grid points in the higher order rule, not the sum of the number of grid points of both rules.

2 Gaussian Quadrature

Let $P_n(x)$ be the degree-n polynomial which is orthogonal to all polynomials of lesser degree, i.e.

$$\int_{-1}^{1} P_n(x)p(x)dx = 0 \tag{2}$$

for all $p(x)$ of degree $< n$. With normalization $P_n(1) = 1$, this is defined uniquely and referred to as the n^{th} Legendre polynomial. Let $\{x_i\}_{i=1}^n$ denote the n roots of $P_n(x)$. All of these roots are contained in $(-1, 1)$. To see this, let

$x_1, ..., x_k$ be all of the points in $(-1, 1)$ where $P_n(x)$ crosses zero (and changes sign). We prove by contradiction that $k = n$. Suppose $k < n$, then define

$$p(x) := (x - x_1) \cdots (x - x_k) \tag{3}$$

which has simple roots (that change sign) at the x_j's. Then the product $P_n(x)p(x)$ does not change sign at the x_j's. Since neither function changes sign anywhere else, we conclude that the product is of the same sign across the domain. Therefore

$$\int_{-1}^{1} P_n(x)p(x)dx \neq 0 \tag{4}$$

but this violates the assumption that $P_n(x)$ is orthogonal to all lower degree polynomials. Therefore $k = n$. $\square$

The n-point Gauss-Legendre quadrature rule on $(-1, 1)$ is then given by

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i), \tag{5}$$

where

$$w_i := \frac{2}{(1 - x_i^2)P_n'(x_i)^2} \tag{6}$$

This is exact for all polynomials of degree less than or equal to $2n-1$. Note that a general n-point quadrature rule can be made to be exact for polynomials of degree $\leq n - 1$ by choosing certain weights. Let $q(x)$ be a polynomial of degree $\leq 2n - 1$ and do polynomial long-division by P_n:

$$q(x) = P_n(x)p(x) + r(x) \tag{7}$$

where $p(x)$ has degree $\leq n - 1$ and $r(x)$ has degree $\leq n - 1$. Then observe that

$$\int_{-1}^{1} q(x)dx = \int_{-1}^{1} r(x)dx \tag{8}$$

and

$$\sum_{i=1}^{n} w_i q(x_i) = \sum_{i=1}^{n} w_i r(x_i) \tag{9}$$

and since r has degree less than n, we can choose w_i's to integrate it exactly and thus q has been integrated exactly.

To integrate over an arbitrary interval, the weights and nodes are mapped as follows:

$$\int_{a}^{b} f(x)dx \approx \frac{b-a}{2} \sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right). \tag{10}$$

In our error estimates in Gauss-Kronrod quadrature, this will be our lower-order (or "embedded") rule.

3 Gauss-Kronrod quadrature

In 1964, Aleksandr Kronrod discovered that an n-point Gauss-Legendre quadrature rule can be extended by adding $n+1$ additional nodes to create a quadrature rule that is exact for polynomials of degree $\leq 3n+1$. Let $E_{n+1}(x)$ be the polynomial of degree $n+1$ for which

$$\int_{-1}^{1} P_n(x)E_{n+1}(x)p(x)dx = 0 \tag{11}$$

for all polynomials $p(x)$ of degree $\leq n$. With normalization such that the leading monomial has coefficient 1, this is uniquely determined and is known as the $(n+1)$th **Stieltjes polynomial**. The additional $(n+1)$ nodes are defined to be the roots of $E_{n+1}(x)$, which are all contained in $(-1,1)$. Proof of this fact follows a similar structure to the one in the preceding section for the Legendre nodes. The weights are then chosen to make integration exact for polynomials of degree $\leq 3n+1$. Let K denote this quadrature rule,

$$K[f] := \sum_{i=1}^{2n+1} a_i f(x_i) \tag{12}$$

and G denote the lower-order Gaussian rule,

$$G[f] := \sum_{i=1}^{n} b_i f(x_i). \tag{13}$$

The error of K is approximated by computing the error between K and G:

$$\left| \int_a^b f(x)dx - K[f] \right| \approx |K[f] - G[f]| \tag{14}$$

which requires only $2n+1$ evaluations of f to compute. If a completely unrelated quadrature rule with $2n+1$ nodes had been used as the higher-order rule, then the error approximation would have required $n + (2n+1) = 3n+1$ function evaluations.

As described in the Introduction, GK quadrature is an adaptive rule that integrates over panels, which are split into smaller panels if the error approximation in Equation 14 returns a large number. Julia's QuadGK.jl package implements Gauss-Kronrod quadrature to arbitrary accuracy.