APPENDIX C

GAUSSIAN QUADRATURE

THIS appendix gives a derivation of the fundamental formulas for Gaussian quadrature, which were discussed but not derived in Section 5.6.2.

Gaussian quadrature, defined over the standard domain from -1 to 1, makes use of an integration rule of the form

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \simeq \sum_{k=1}^{N} w_k f(x_k). \tag{C.1}$$

The derivation of the positions x_k of the sample points and the weights w_k is based on the mathematics of Legendre polynomials. The Legendre polynomial $P_N(x)$ is an Nth-order polynomial in x that has the property

$$\int_{-1}^{1} x^k P_N(x)\,\mathrm{d}x = 0 \qquad \text{for all integer } k \text{ in the range } 0 \le k < N \tag{C.2}$$

and satisfies the normalization condition

$$\int_{-1}^{1} \bigl[P_N(x)\bigr]^2\,\mathrm{d}x = \frac{2}{2N+1}. \tag{C.3}$$

Thus, for instance, $P_0(x) =$ constant, and the constant is fixed by (C.3) to give $P_0(x) = 1$. Similarly, $P_1(x)$ is a first-order polynomial $ax + b$ satisfying

$$\int_{-1}^{1} (ax + b)\,\mathrm{d}x = 0. \tag{C.4}$$

Carrying out the integral, we find that $b = 0$ and a is fixed by (C.3) to be 1, giving $P_1(x) = x$. The next two polynomials are $P_2(x) = \frac{1}{2}(3x^2 - 1)$ and $P_3(x) = \frac{1}{2}(5x^3 - 3x)$, and you can find tables on-line or elsewhere that list them to higher order.

Now suppose that $q(x)$ is a polynomial of degree less than N, so that it can be written $q(x) = \sum_{k=0}^{N-1} c_k x^k$ for some set of coefficients c_k. Then

$$\int_{-1}^{1} q(x) P_N(x)\,\mathrm{d}x = \sum_{k=0}^{N-1} c_k \int_{-1}^{1} x^k P_N(x)\,\mathrm{d}x = 0, \tag{C.5}$$

by Eq. (C.2). Thus, for any N, $P_N(x)$ is orthogonal to every polynomial of lower degree. A further property of the Legendre polynomials, which we will use shortly, is that for all N the polynomial $P_N(x)$ has N real roots that all lie in the interval from -1 to 1. That is, there are N values of x in this interval for which $P_N(x) = 0$.

Returning now to our integral, Eq. (C.1), suppose that the integrand $f(x)$ is a polynomial in x of degree $2N-1$ or less. If we divide $f(x)$ by the Legendre polynomial $P_N(x)$, then we get

$$f(x) = q(x)P_N(x) + r(x), \tag{C.6}$$

where $q(x)$ and $r(x)$ are both polynomials of degree $N-1$ or less. Thus our integral can be written

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \int_{-1}^{1} q(x)P_N(x)\,\mathrm{d}x + \int_{-1}^{1} r(x)\,\mathrm{d}x = \int_{-1}^{1} r(x)\,\mathrm{d}x, \tag{C.7}$$

where we have used (C.5). This means that to find the integral of the polynomial $f(x)$ we have only to find the integral of the polynomial $r(x)$, which always has degree $N-1$ or less.

But we already know how to solve this problem. As we saw in Section 5.6.1, for any choice of sample points x_k a polynomial of degree $N-1$ or less can be fitted exactly using the interpolating polynomials $\phi_k(x)$, Eq. (5.49), and then the fit can be integrated to give a formula of the form

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \int_{-1}^{1} r(x)\,\mathrm{d}x = \sum_{k=1}^{N} w_k r(x_k), \tag{C.8}$$

where

$$w_k = \int_{-1}^{1} \phi_k(x)\,\mathrm{d}x. \tag{C.9}$$

(See Eq. (5.56) on page 163.) Note that, unlike Eq. (C.1), the equality in Eq. (C.8) is now an exact one (because the fit is exact).

Thus we have a method for integrating any polynomial of order $2N-1$ or less exactly over the interval from -1 to 1: we divide by the Legendre polynomial $P_N(x)$ and then integrate the remainder polynomial $r(x)$ using any set of N sample points we choose plus the corresponding weights.

This, however, is not a very satisfactory method. In particular the polynomial division is rather complicated to perform. However, we can simplify the procedure by noting that, so far, the positions of our sample points are unconstrained and we can pick them in any way we please. So consider again an

integration rule of the form (C.1) and make the substitution (C.6), to get

$$\sum_{k=1}^{N} w_k f(x_k) = \sum_{k=1}^{N} w_k q(x_k) P_N(x_k) + \sum_{k=1}^{N} w_k r(x_k). \tag{C.10}$$

But we know that $P_N(x)$ has N zeros between -1 and 1, so let us choose our N sample points x_k to be exactly the positions of these zeros. That is, let x_k be the kth root of the Legendre polynomial $P_N(x)$. In that case, $P_N(x_k) = 0$ for all k and Eq. (C.10) becomes simply

$$\sum_{k=1}^{N} w_k f(x_k) = \sum_{k=1}^{N} w_k r(x_k). \tag{C.11}$$

Combining with Eq. (C.8), we then have

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \sum_{k=1}^{N} w_k f(x_k), \tag{C.12}$$

where the equality is an exact one.

Thus we have a integration rule of the standard form that allows us to integrate any polynomial function $f(x)$ of order $2N-1$ or less from -1 to 1 and get an *exact* answer (except for rounding error). It will give the exact value for the integral, even though we only measure the function at N different points.

We have not derived the closed-form expression for the weights w_k given in Eq. (5.60). The derivation of this expression is lengthy and tedious, so we omit it here, but the enthusiastic reader can find it in Hildebrand, F. B., *Introduction to Numerical Analysis*, McGraw-Hill, New York (1956).

GAUSS–KRONROD QUADRATURE

A widely used variant of Gaussian quadrature is *Gauss–Kronrod quadrature*, which was mentioned briefly, but not defined, in Section 5.6.3. Gauss–Kronrod quadrature provides an additional set of sample points interlaced between those of ordinary Gaussian quadrature. By computing an estimate of an integral using just the ordinary Gaussian points, and then recomputing it using the two sets of points combined, one gets two values whose difference gives an estimate of the error on the result. Thus Gauss–Kronrod quadrature gives results of accuracy comparable with Gaussian quadrature plus an estimate of the error on the result (which Gaussian quadrature alone does not provide), but does so at the expense of some addition computational effort, since one must evaluate the integrand at all of the additional sample points.

The derivation of the Gauss–Kronrod formula is similar to that for ordinary Gaussian quadrature. Suppose we choose N sample points to be the roots of the Nth Legendre polynomial $P_N(x)$, as in standard Gaussian quadrature, and an additional $N+1$ other points, which we are free to place anywhere we like, for a total of $2N+1$ points. For any integrand $f(x)$ we can create a polynomial approximation of degree $2N$ that matches the integrand exactly at these $2N+1$ points, for instance using the method of interpolating polynomials from Section 5.6.1, then integrate that approximation to get an approximation to the integral of $f(x)$. If $f(x)$ itself happens to be a polynomial of degree $2N$ or less, then the calculation will be exact, apart from rounding error.

But now we note that we have $N+1$ degrees of freedom in the positions of our additional $N+1$ sample points, which as we have said we can choose in any way we like, and this suggests that, if we choose those points correctly, we should be able to create an integration rule that is exact for polynomials of degree $N+1$ higher, i.e., polynomials of degree $3N+1$. Gauss–Kronrod quadrature tells us how to pick the additional $N+1$ points to achieve this. The result is an integration rule with $2N+1$ sample points that is accurate for polynomials up to degree $3N+1$, which is not as good as Gaussian quadrature (which would be accurate up to degree $4N+1$ on $2N+1$ points), but it's the best we can do if we restrict our first N points to fall at the roots of $P_N(x)$.

To describe this another way, the N initial points at the roots of $P_N(x)$ are *nested* within (i.e., a subset of) the $2N+1$ points for the Gauss–Kronrod quadrature, which is the crucial property that makes Gauss–Kronrod quadrature attractive. It means we can evaluate our integral using standard Gaussian quadrature on N points, and then again using Gauss–Kronrod quadrature on $2N+1$, as described above, and the second calculation requires us to evaluate the integrand $f(x)$ only at the newly added sample points. For the rest of the points we can reuse the values from the first step. (Notice, however, that the weights w_k for the quadrature rule are different on the two steps, so one must recompute the sum, Eq. (C.1). One can reuse values of $f(x)$ on the second step, which can save a lot of time, but one cannot reuse the value of the complete sum.)

How then do we choose the additional $N+1$ sample points for Gauss–Kronrod quadrature? Let us define a new polynomial $E_{N+1}(x)$ of degree $N+1$ by

$$\int_{-1}^{1} x^k P_N(x) E_{N+1}(x)\,\mathrm{d}x = 0, \quad \text{for integer } k \text{ in the range } 0 \le k \le N. \tag{C.13}$$

This formula gives us $N+1$ conditions on $E_{N+1}(x)$. If we also fix the nor-

malization of $E_{N+1}(x)$ (using any method we like), then we have $N+2$ conditions, which is enough to fix all $N+2$ coefficients of the polynomial and hence uniquely specify it. The polynomials $E_N(x)$ are known as *Stieltjes polynomials*. In Gauss–Kronrod quadrature, we choose the additional $N+1$ sample points to be the roots of the polynomial $E_{N+1}(x)$. Thus the complete set of $2N+1$ sample points is the set of roots of $P_N(x)$ plus the roots of $E_{N+1}(x)$. The corresponding integration weights w_k can then be calculated using Eq. (5.56) on page 163.

Now suppose our integrand $f(x)$ is a polynomial of degree $3N+1$ or less. If we divide $f(x)$ by $P_N(x)E_{N+1}(x)$—which is a polynomial of degree $2N+1$—we get

$$f(x) = q(x)P_N(x)E_{N+1}(x) + r(x), \tag{C.14}$$

where $q(x)$ and $r(x)$ are polynomials of degree N or less. Then the integral of $f(x)$ over the standard interval from -1 to 1 is

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \int_{-1}^{1} q(x)P_N(x)E_{N+1}(x)\,\mathrm{d}x + \int_{-1}^{1} r(x)\,\mathrm{d}x = \int_{-1}^{1} r(x)\,\mathrm{d}x, \tag{C.15}$$

where we have used (C.13) to eliminate the first term. This integral can now be evaluated in the standard fashion

$$\int_{-1}^{1} r(x)\,\mathrm{d}x = \sum_{k=1}^{2N+1} w_k r(x_k), \tag{C.16}$$

where, as we have said, the sample points x_k are the roots of the Legendre and Stieltjes polynomials. Since $r(x)$ is a polynomial of order N or less and there are $2N+1$ sample points, Eq. (C.16) will always give an exact answer, to the limits set by rounding error.

But now, using Eq. (C.14), we can also write

$$\begin{aligned}\sum_{k=1}^{2N+1} w_k f(x_k) &= \sum_{k=1}^{2N+1} w_k q(x_k)P_N(x_k)E_{N+1}(x_k) + \sum_{k=1}^{2N+1} w_k r(x_k)\\ &= \sum_{k=1}^{2N+1} w_k r(x_k),\end{aligned} \tag{C.17}$$

where the first sum has vanished because every sample point x_k falls at a zero of either $P_N(x)$ or $E_{N+1}(x)$, so every term in the sum is zero. Combining Eqs. (C.15) to (C.17), we have

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \sum_{k=1}^{2N+1} w_k f(x_k), \tag{C.18}$$

where the equality is an exact one. Thus this particular choice of sample points does indeed give us an integration rule that is exact for all polynomial integrands of order $3N + 1$ or less.

The Gauss–Kronrod integration method now involves the following steps:

1. We evaluate the integral of $f(x)$ first using standard Gaussian quadrature on N points.
2. We evaluate it again using Gauss–Kronrod quadrature on $2N + 1$ points. N of those points are the same as those for Gaussian quadrature—the roots of $P_N(x)$—so we do not have to recalculate $f(x)$ at these points. We can reuse the values from step 1. Only the values at the $N + 1$ new points have to be calculated, and this can save us a lot of time.
3. The second estimate of the integral (since it is the more accurate of the two) gives us our final result. And the difference between the two estimates gives us an estimate of the error, by analogy with Eq. (5.62). In fact, the difference only gives us an upper bound on the error. The actual error is probably significantly smaller, but unfortunately no precise expression for the error is known, so in practice one usually just uses the difference, bearing in mind that the true error may in fact be smaller than this.