Appendix C

Gaussian quadrature

This appendix gives a derivation of the fundamental results of Gaussian quadrature, which were discussed but not derived in Section 5.5.2.

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

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

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 5.5.1, for any choice of sample points x_k a polynomial of degree $n-1$ or less can be fitted exactly and uniquely using the interpolating polynomials, Eq. (5.43), 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, unlike Eq. (C.1), the equality is now an exact one (because the fit is exact and unique).

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 $r(x)$ exactly 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

$$\sum_{k=1}^{n} w_k f(x_k) = \sum_{k=1}^{n} w_k q(x_k) P_n(x_k) + \sum_{k=1}^{n} w_k r(x_k). \tag{C.9}$$

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.9) becomes simply

$$\sum_{k=1}^{n} w_k f(x_k) = \sum_{k=1}^{n} w_k r(x_k). \tag{C.10}$$

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

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \sum_{k=1}^{n} w_k f(x_k), \tag{C.11}$$

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. (5.54). The derivation of this expression is lengthy and tedious, so we omit it here. The enthusiastic reader can find it in Hildebrand, F. B., *Introduction to Numerical Analysis*, McGraw-Hill, New York (1956).