LECTURE NOTES
COMPUTATIONAL METHODS FOR MACROECONOMICS
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KAREN A. KOPECKY

Numerical Integration

Numerical integration methods or quadrature methods are used to approximate integrals. We need these techniques when we are unable to compute an integral analytically. Suppose we are interested in computing the integral of some function $f(x)$ over the interval $[a, b]$. The basic idea of numerical quadrature is to approximate the integral by a weighted sum of function evaluations, or

$$\int_a^b f(u)du = \sum_{i=1}^{n} \omega_i f(x_i) + \epsilon, \tag{1}$$

where ϵ is the approximation error. Three issues (at least) are important here.

1. Choice of the quadrature nodes that is the x_i's.
2. Choice of the quadrature weights, that is the ω_i's.
3. Choice of the number of function evaluations: n.

There is no general recipe for making these choices since what a good choice is will vary depending on the problem. If, for instance, the function is not difficult to evaluate, choosing a large n is not a problem. If, on the contrary, the function is not easily computable, then one might want to limit the number of function evaluations, and make up for that by choosing nodes and weights more carefully. As with most numerical procedures, when choosing n we are confronted with the standard trade-off between efficiency and precision. Also note, that these methods can be extended to computing multi-dimensional integrals in a straightforward way by computing nodes and weights along each dimension and and taking as the tensor products of the sets.

1 Newton-Cotes formula

The classical numerical integration formulas, or Newton-Cotes formulas are based on the following idea:

> Break the interval of interest up into n equally spaced subintervals. Then, approximate f over these subintervals with a low-order polynomial. Finally, use the integral of the polynomial over the subinterval as an approximation of the integral of f over the subinterval.

Approximating f with constant functions yields the midpoint rule. Approximating f with linear functions delivers the trapezoid rule. Approximating with quadratics delivers Simpson's rule of integration. One can of course use higher degree polynomials to improve the accuracy of the estimated interval.

1.1 Midpoint rule

Suppose we break the interval $[a, b]$ into n equally spaced subintervals. Each subinterval will have length $h \equiv (b - a)/n$. Denote by x_i the midpoint of interval i. If we approximate $f(x)$ on interval i by the zero-order Taylor expansion of f about x_i we obtain the following approximation to the integral of f on interval i:

$$\int_{x_i - \frac{h}{2}}^{x_i + \frac{h}{2}} f(x)dx \approx \int_{x_i - \frac{h}{2}}^{x_i + \frac{h}{2}} f(x_i)dx = f(x_i)h. \tag{2}$$

Thus we can derive an approximation to the integral over $[a, b]$,

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} f(x_i)h. \tag{3}$$

Basically we are approximating the integral by the sum of the area of n rectangles of height $f(x_i)$ and length h.

When trying to determine which method to use one important consideration is the size of the approximation error incurred. Hence we will now derive an upper bound on this error under the midpoint rule. First define $F(x) \equiv \int f(x)dx$ so that

$$\int_{x_i - \frac{h}{2}}^{x_i + \frac{h}{2}} f(x)dx = F(x_i + \frac{h}{2}) - F(x_i - \frac{h}{2}).$$

Then plugging the interval endpoints into a third-order Taylor expansion of $F(\cdot)$ about x_i and applying Taylor's Remainder Theorem yields

$$F(x_i + \frac{h}{2}) = F(x_i) + \frac{h}{2}F'(x_i) + \frac{1}{2}\left(\frac{h}{2}\right)^2 F''(x_i) + \frac{1}{6}\left(\frac{h}{2}\right)^3 F'''(\zeta_{1i}), \quad (4)$$

$$F(x_i - \frac{h}{2}) = F(x_i) - \frac{h}{2}F'(x_i) + \frac{1}{2}\left(\frac{h}{2}\right)^2 F''(x_i) - \frac{1}{6}\left(\frac{h}{2}\right)^3 F'''(\zeta_{2i}), \quad (5)$$

for $\zeta_{1i} \in [x_i, x_i + h/2]$ and $\zeta_{2i} \in [x_i - h/2, x_i]$. Thus

$$\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} f(x)dx = F(x_i + \frac{h}{2}) - F(x_i - \frac{h}{2}) = hF'(x_i) + \frac{h^3}{48}(F'''(\zeta_{1i}) + F'''(\zeta_{2i})) \quad (6)$$

$$= hf(x_i) + \frac{h^3}{48}(f''(\zeta_{1i}) + f''(\zeta_{2i})). \quad (7)$$

So

$$\int_a^b f(x)dx = \sum_{i=1}^{n} \int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} f(x)dx = \sum_{i=1}^{n} hf(x_i) + \sum_{i=1}^{n} \frac{h^3}{48}(f''(\zeta_{1i}) + f''(\zeta_{2i})) \quad (8)$$

which means the approximation error, ε, is

$$\varepsilon = \left| \sum_{i=1}^{n} \frac{h^3}{48}(f''(\zeta_{1i}) + f''(\zeta_{2i})) \right| \leq \frac{h^3}{48} 2nM = \frac{h^2}{24}(b-a)M, \quad (9)$$

where $M = \max_{[a,b]} |f''(x)|$ and remembering that $(b - a) = nh$. Notice that the error converges quadratically in h.

2 Gaussian Quadrature

Let's consider the more general problem of approximating the integral of a real-valued function f with respect to a *weight function* ω over the interval $[a, b]$, i.e., of approximating

$$I(f) := \int_a^b f(x)\omega(x)dx.$$

Note the interval $[a, b]$ may be infinite, such as $[0, +\infty]$ or $[-\infty, +\infty]$. The weight function must satisfy the following

(a) $\omega \geq 0$ is measurable on the finite or infinite interval $[a, b]$.

(b) All moments $\mu_k = \int_a^b x^k \omega(x)dx$, $k = 0, 1, \ldots,$ exist and are finite.

(c) For polynomials $s(x)$ which are nonnegative on $[a,b]$, $\int_a^b \omega(x)s(x)dx = 0$ implies $s(x) = 0$ for all x or equivalently $\int_a^b \omega(x)dx > 0$.

If $\omega(x)$ is positive and continuous on the finite interval $[a,b]$ then these conditions would be met.

2.1 Basic Idea

We are still interested in finding approximations of the form

$$\tilde{I}(f) := \sum_{i=1}^{n} w_i f(x_i).$$

When we use Newton-Cotes formulas we fix the location of the nodes, and focus on choosing the weights. But there may be a better choice for the location of the nodes than evenly-space along the interval. With Gaussian quadrature we choose both the nodes and the weights to maximize the degree of polynomial for which $I(f)$ and $\tilde{I}(f)$ coincide.

Remember the definition of an inner product with respect to the weighting function ω. Given two functions f and g defined on at least $[a,b]$ their inner product is given by

$$\langle f, g\rangle := \int_a^b f(x)g(x)w(x)dx.$$

If $\langle f, g\rangle = 0$ then f and g are said to be orthogonal.

Define $\bar{\Pi}_j$ to be the set of all real polynomials of degree j, i.e.,

$$\bar{\Pi}_j := \{p|\text{degree}(p) = j\}$$

and Π_j to be the set of all real polynomials with degree less than or equal to j, or

$$\Pi_j := \{p|\text{degree}(p) \leq j\}.$$

The following theorem proves the existence of a sequence of mutually orthogonal polynomials with respect to the weighting function ω.

Theorem 1. *There exists polynomials $p_j \in \bar{\Pi}_j$, $j = 0, 1, \ldots,$ such that*

$$\langle p_i, p_k\rangle = 0 \quad \textit{for} \quad i \neq k$$

and these polynomials are uniquely defined by the recursions

$$p_0(x) \equiv 1,$$

$$p_{i+1}(x) \equiv (x - \delta_{i+1})p_i(x) - \gamma_{i+1}^2 p_{i-1}(x), \quad \textit{for } i \geq 0,$$

where $p_{-1}(x) :\equiv 0$ *and*

$$\delta_{i+1} := \langle xp_i, p_i \rangle / \langle p_i, p_i \rangle \quad \textit{for } i \geq 0,$$

$$\gamma_{i+1}^2 := \begin{cases} 1 & \textit{for } i = 0, \\ \langle p_i, p_i \rangle / \langle p_{i-1}, p_{i-1} \rangle & \textit{for } i \geq 1. \end{cases}$$

The proof is omitted but goes as follows. The polynomials can be constructed recursively using the *Gram-Schmidt orthogonalization* technique. Clearly the theorem holds for $j = 0$. The proof follows by induction.

Every polynomial $p \in \Pi_k$ can be represented as a linear combination of the orthogonal polynomials p_i, $i \leq k$. It follows that the inner product of any polynomial p of degree less than n with the nth degree orthogonal polynomial must be 0.

Corollary 2. $\langle p, p_n \rangle = 0$ *for all* $p \in \Pi_{n-1}$.

Theorem 3. *The roots* z_i*,* $i = 1, \ldots, n$ *of* p_n *are real and simple. They all lie in the open interval* (a, b).

Proof. Take those roots of p_n which lie in (a, b) and at which p_n changes sign:

$$a < z_1 < \cdots < z_m < b$$

Construct a polynomial

$$q(z) := \prod_{j=1}^{m} (z - z_j) \in \bar{\Pi}_m$$

Note that $q(z)$ is such that $p_n(z)q(z)$ does not change sign in $[a, b]$. Thus

$$\langle p_n, q \rangle = \int_a^b \omega(z) p_n(z) q(z) dz \neq 0$$

and degree$(q) = m = n$ must hold since otherwise $\langle p_n, q \rangle = 0$. □

Theorem 4. *The* $n \times n$ *matrix*

$$A := \begin{bmatrix} p_0(x_1) & \cdots & p_0(x_n) \\ \vdots & & \vdots \\ p_{n-1}(x_1) & \cdots & p_{n-1}(x_n) \end{bmatrix}$$

is nonsingular for mutually distinct arguments x_i, $i = 1, \ldots, n$.

Proof. Assume A is singular. Then there is a vector $c^T = (c_0, \ldots, c_{n-1})$ with $c \neq 0$ and $c^T A = 0$. The polynomial

$$q(x) := \sum_{i=0}^{n-1} c_i p_i(x)$$

must have degree$(p) < n$ but has n distinct roots $x_1, \ldots, x_n$ so $q(x) \equiv 0$. Since the polynomials p_i, $i = 0, \ldots, n-1$ are linearly independent it must be that $c = 0$, a contradiction. □

Theorem 4 shows that the interpolation problem always has a solution.

Theorem 5. *(a) Let* $z_1, \ldots, z_n$ *be the roots of the* n*th orthogonal polynomial* $p_n(x)$*, and let* $w_1, \ldots, w_n$ *be the solution of the (nonsingular) system of equations*

$$\sum_{i=1}^{n} p_k(z_i) w_i = \begin{cases} \langle p_0, p_0 \rangle & \text{if} \quad k = 0, \\ 0 & \text{if} \quad k = 1, 2, \ldots, n-1. \end{cases} \tag{10}$$

Then $w_i > 0$ *for* $i = 1, 2, \ldots, n$ *and*

$$\int_a^b w(x) p(x) dx = \sum_{i=1}^{n} w_i p(z_i) \tag{11}$$

holds for all polynomials $p \in \Pi_{2n-1}$*. The positive numbers* w_i *are called "weights".*

(b) conversely, if the numbers w_i*,* z_i*,* $i = 1, \ldots, n$ *are such that* (11) *holds for all* $p \in \Pi_{2n-1}$*, then the* z_i *are the roots of* p_n *and the weights* w_i *satisfy* (10)*.*

(c) It is not possible to find numbers z_i*,* w_i*,* $i = 1, \ldots, n$ *such that* (11) *holds for all polynomials* $p \in \Pi_{2n}$*.*

Proof. By theorem 3, the roots z_i, $i = 1, \ldots, n$ of p_n are real and mutually distinct number in (a, b). By theorem 4, the matrix

$$A := \begin{bmatrix} p_0(z_1) & \cdots & p_0(z_n) \\ \vdots & & \vdots \\ p_{n-1}(z_1) & \cdots & p_{n-1}(z_n) \end{bmatrix}$$

is nonsingular and the system of equations (10) has a unique solution.

Take an arbitrary polynomial $p \in \Pi_{2n-1}$. It can be written in the form

$$p(x) \equiv p_n(x)q(x) + r(x) \tag{12}$$

where q and r are polynomials in Π_{n-1}. Hence we can express them as linear combinations of orthogonal polynomials

$$q(x) \equiv \sum_{k=0}^{n-1} \alpha_k p_k(x)$$

and

$$r(x) \equiv \sum_{k=0}^{n-1} \beta_k p_k(x).$$

We can now write the left-hand-side of 11 as

$$\begin{aligned}
\int_a^b \omega(x)p(x)dx &= \int_a^b \omega(x)p_n(x)q(x)dx + \int_a^b \omega(x)r(x)dx \\
&= \langle p_n, q\rangle + \langle r, p_0\rangle \\
&= \beta_0\langle p_0, p_0\rangle
\end{aligned}$$

where the middle line follows from the fact that $p_0(x) \equiv 1$ and the last line follows from corollary 2.

The right-hand-side of (11) is

$$\begin{aligned}
\sum_{i=1}^{n} w_i p(z_i) &= \sum_{i=1}^{n} w_i r(z_i) \\
&= \sum_{k=0}^{n-1} \beta_k \left(\sum_{i=1}^{n} w_i p_k(z_i)\right) \\
&= \beta_0\langle p_0, p_0\rangle
\end{aligned}$$

where the first line follows from $p_n(z_i) = 0$, the third line follows from (10). So (11) holds.

We will now show that if w_i and z_i for $i = 1, \ldots, n$ are such that (11) holds for all polynomials $p \in \Pi_{2n-1}$ then $w_i > 0$ for $i = 1, \ldots, n$. Apply (11) to the polynomials

$$\bar{p}_j(x) := \prod_{h=1, h\neq j}^{n} (x - z_h)^2 \in \Pi_{2n-2}, \quad j = 1, \ldots, n,$$

and note that by the definition of the weighting function

$$0 < \int_a^b \omega(x)\bar{p}_j(x)dx = \sum_{i=1}^{n} w_i \bar{p}_j(z_i) = w_j \prod_{h=1, h\neq j}^{n} (z_j - z_h)^2$$

That completes the proof of part (a).

Now we'll prove part (c). Take

$$\bar{p}(x) :\equiv \prod_{j=1}^{n}(x - z_j)^2 \in \Pi_{2n}$$

If (11) holds for $\bar{p}(x)$ then

$$0 < \int_a^b \omega(x)\bar{p}(x)dx = \sum_{i=1}^{n} w_i \bar{p}(z_i) = 0$$

But this can't be.

Finally we will prove part (b). Suppose that w_i, z_i, $i = 1, \ldots, n$ are such that (11) holds for all $p \in \Pi_{2n-1}$. First note that the abscissas z_i must be mutually distinct, since otherwise we could formulate the same integration rule using only $n-1$ of the abscissas x_i, and this would contradict part (c).

Apply (11) to the orthogonal polynomials $p = p_k$, $k = 0, \ldots, n-1$ and we obtain

$$\begin{aligned} \sum_{i=1}^{n} w_i p_k(x_i) &= \int_a^b \omega(x) p_k(x) dx, \\ &= \langle p_k, p_0 \rangle, \\ &= \begin{cases} \langle p_0, p_0 \rangle, & \text{if } k = 0, \\ 0, & \text{if } 1 \le k \le n-1. \end{cases} \end{aligned}$$

So the weights w_i must satisfy (10).

Apply (11) to $p(x) :\equiv p_k(x)p_n(x)$, $k = 0, \ldots, n-1$, and we obtain

$$\sum_{i=1}^{n} w_i p_n(z_i) p_k(z_i) = \langle p_k, p_n \rangle = 0, \quad k = 0, \ldots, n-1.$$

Where the last equality follows from corollary 2. This means that the vector $c = (w_1 p_n(z_1), \ldots, w_n p_n(z_n))^T$ solves the homogeneous system of equations $Ac = 0$. Since the abscissas z_i are mutually distinct, the matrix A is nonsingular by theorem 4. So $c = 0$ and $w_i p_n(z_i) = 0$, for $i = 1, \ldots, n$. Since if (11) holds then $w_i > 0$ for $i = 1, \ldots, n$ was shown in the proof for part (a), we have $p_n(x_i) = 0$, $i = 1, \ldots, n$.

□

Note that the w_i,$i = 1, \ldots, n$ that solve (10) should be also be the solutions to

$$w_i = \int_a^b l_i(x)\omega(x)dx, \quad i = 1, n.$$

2.2 Gauss-Legendre Quadrature

If the weighting function is $\omega(x) = 1$ and the interval is $[-1, 1]$ then the corresponding orthogonal polynomials are the Legendre polynomials,

$$L_k(x) = \frac{k!}{(2k)!}\frac{d^k}{dx^k}(x^2-1)^k, \quad k = 0, 1, \ldots$$

We choose as our $\{z_i\}_{i=1}^n$ the roots of the nth Legendre polynomial. The weights solve (10) and our approximation to

$$I(f) = \int_{-1}^{1} f(x)dx,$$

is

$$\tilde{I}(f) = \sum_{i=1}^{n} w_i f(z_i).$$

Suppose we want to approximate the integral of

$$I(f) = \int_{a}^{b} f(x)dx.$$

To do this we need to do a change of variables. Define g to be the linear mapping from $[-1, 1]$ to $[a, b]$ such that $g(-1) = a$ and $g(1) = b$ then

$$\int_{a}^{b} f(x)dx = \int_{-1}^{1} f(g(z))g'(z)dz.$$

So our approximation is

$$\tilde{I}(f) = \sum_{i=1}^{n} w_i f(g(z_i))g'(z_i).$$

2.3 Gauss-Chebyshev Quadrature

If the weighting function is $\omega(x) = (1-x^2)^{-1/2}$ and the interval is $[-1, 1]$ then the corresponding orthogonal polynomials are the Chebyshev polynomials,

$$T_k(x) \quad = \quad \cos(k\cos^{-1}(x)), \quad k = 0, 1, \ldots.$$

We choose as our $\{z_i\}_{i=1}^n$ the roots of the nth Chebyshev polynomial. The weights turn out to be $w_i = \pi/n$ for $i = 1, \ldots, n$ and our approximation to

$$I(f) = \int_{-1}^{1} f(x)\omega(x)dx,$$

is

$$\tilde{I}(f) = \sum_{i=1}^{n} w_i f(z_i).$$

Suppose we are interested in approximating

$$I(f) = \int_a^b f(x)dx,$$

using Gauss-Chebyshev quadrature. We can do the following

$$\begin{aligned}\int_a^b f(x)dx &= \int_{-1}^{1} f(g(z))g'(z)dz, \\ &= \int_{-1}^{1} \frac{f(g(z))g'(z)}{\omega(z)}\omega(z)dz, \\ &= \int_{-1}^{1} h(z)\omega(z)dz.\end{aligned}$$

So

$$\tilde{I}(f) = \sum_{i=1}^{n} w_i h(z_i).$$

2.4 Gauss-Hermite Quadrature

If the weighting function is $\omega(x) = e^{-x^2}$ and the interval is $[-\infty, \infty]$ then the corresponding orthogonal polynomials are the Hermite polynomials,

$$H_k(x) = (-1)^k e^{x^2} \frac{d^k}{dx^k} e^{-x^2}, \quad k = 0, 1, \ldots.$$

We choose as our $\{z_i\}_{i=1}^n$ the roots of the nth Hermite polynomial. The weights solve (10) and our approximation to

$$I(f) = \int_{-\infty}^{\infty} f(x)\omega(x)dx,$$

is

$$\tilde{I}(f) = \sum_{i=1}^{n} w_i f(z_i).$$

This is useful for computing integrals involving the normal distribution. For example suppose we want to compute $E[f(x)]$ where $x \sim N(\mu, \sigma^2)$. We need to compute

$$E[f(x)] = \int_{-\infty}^{\infty} f(x) \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\left(\frac{x-\mu}{\sqrt{2}\sigma}\right)^2\right] dx$$

Let

$$z = \frac{x-\mu}{\sqrt{2}\sigma}$$

so that

$$x = \sqrt{2}\sigma z + \mu$$

and $dx = \sqrt{2}\sigma dz$, then

$$\begin{aligned} E[f(x)] &= \int_{-\infty}^{\infty} f(\sqrt{2}\sigma z + \mu) \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-z^2\right] \sqrt{2}\sigma dz \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(\sqrt{2}\sigma z + \mu) e^{-z^2} dz. \end{aligned}$$

and

$$\widetilde{E}[f(x)] = \frac{1}{\sqrt{\pi}} \sum_{i=1}^{n} f(\sqrt{2}\sigma z_i + \mu) w_i.$$

Source:

- **Stoer, J. and R. Bulirsch** 2002. *Introduction to Numerical Analysis.* Springer-Verlag New York, Inc.