Numerical Differentiation and Integration

Econ 5170

Computational Methods in Economics

2022-2023 Spring

Outline

1. Numerical Differentiation
2. Numerical Integration
   - Newton-Cotes Formulas
   - Gaussian Formulas
   - Multidimensional Integration

Numerical Differentiation

- One-sided formula

$$f'(x) \doteq \frac{f(x+h) - f(x)}{h}$$

- What should h be in light of computer errors?
- Error Analysis when $\hat{f}$ is computer version of f
  - Suppose $|f(x) - \hat{f}(x)| \leq \varepsilon$,
  - Actual machine approximation is

$$D(h) = \frac{\hat{f}(x+h) - \hat{f}(x)}{h}$$

  - Error bound is

$$\left| D(h) - \frac{f(x+h) - f(x)}{h} \right| \leq \frac{2\varepsilon}{h}$$

Numerical Differentiation

- Taylor's theorem: for some $\xi \in [x, x+h]$

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi)$$

- If $M_2 > 0$ is an upper bound on $|f''|$ near x,

$$\left| f'(x) - D(h) \right| \leq \frac{2\varepsilon}{h} + \frac{h}{2} M_2$$

- Upper bound on error is minimized at

$$h^* = 2\sqrt{\frac{\varepsilon}{M_2}}$$

- The upper bound on error equals $2\sqrt{\varepsilon M_2}$.

Numerical Differentiation

- Two-Sided Difference Formula
  - Two-sided formula

$$f'(x) \doteq \frac{f(x+h) - f(x-h)}{2h}$$

  - Error is $\frac{h^2}{6}\ f'''(\xi)$ for some $\xi \in [x-h, x+h]$.
  - Round-off error of the approximation error is ε/h
  - Total error of

$$\frac{M_3 h^2}{6} + \frac{\varepsilon}{h}$$

    if $M_3 > |f'''|$ near x.
  - Optimal h is $\frac{3\varepsilon}{M_3}^{1/3}$ with error upper bound of $2\varepsilon^{2/3}\ M_3^{1/3} 9^{1/3}$.
  - Two-sided formula reduced error from order $\varepsilon^{1/2}$ to order $\varepsilon^{2/3}$.

Numerical Differentiation

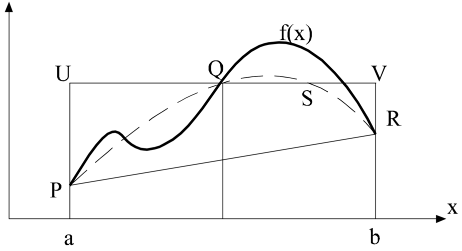
- General Problem
  - Find n-point difference approximation for $f^{(k)}(x)$
  - Optimal step size can be determined by Taylor-series expansions and linear equations.

Integration

- Most integrals cannot be evaluated analytically
- Integrals frequently arise in economics
  - Expected utility
  - Discounted utility and profits over a long horizon
  - Bayesian posterior
  - Likelihood functions
  - Solution methods for dynamic economic models

Newton-Cotes Formulas

- Idea: Approximate function with low order polynomials and then integrate approximation



Newton-Cotes Formulas

- Step function approximation:
  - compute constant function equalling $f(x)$ at midpoint of $[a, b]$
  - Integral approximation is $aUQVb$ box
- Linear function approximation:
  - compute linear function agreeing with $f(x)$ at a and b
  - Integral approximation is trapezoid $aPRb$
- Parabolic function approximation:
  - compute parabola agreeing with $f(x)$ at a, b, and $(a + b)/2$
  - Integral approximation is area of $aPQRb$

Newton-Cotes Formulas

- Midpoint Rule: piecewise step function approximation
  - Simple rule: for some $\xi \in [a, b]$

$$\int_a^b f(x)dx = (b-a)f\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{24}f''(\xi)$$

  - Composite midpoint rule:
    * nodes: $x_j = a + \left(j - \frac{1}{2}\right)h$, $j = 1, 2, \ldots, n$, $h = (b-a)/n$
    * for some $\xi \in [a, b]$

$$\int_a^b f(x)dx = h\sum_{j=1}^{n} f\left(a + \left(j - \frac{1}{2}\right)h\right) + \frac{h^2(b-a)}{24}f''(\xi)$$

Newton-Cotes Formulas

- Trapezoid Rule: piecewise linear approximation
  - Simple rule: for some $\xi \in [a, b]$

$$\int_a^b f(x)dx = \frac{b-a}{2}[f(a) + f(b)] - \frac{(b-a)^3}{12} f''(\xi)$$

  - Composite trapezoid rule:
    * nodes: $x_j = a + (j - \frac{1}{2})h,\ j = 1, 2, \ldots, n,\ h = (b-a)/n$
    * for some $\xi \in [a, b]$

$$\begin{aligned}\int_a^b f(x)dx =& \frac{h}{2}\left[f_0 + 2f_1 + \cdots + 2f_{n-1} + f_n\right] \\ & - \frac{h^2(b-a)}{12} f''(\xi)\end{aligned}$$

- Simpson's Rule: piecewise quadratic approximation
  - for some $\xi \in [a, b]$

$$\int_a^b f(x)dx = \left(\frac{b-a}{6}\right)\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

  - Composite Simpson's rule: for some $\xi \in [a, b]$

$$\int_a^b f(x)dx = \frac{h}{3}\left[f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots + 4f_{n-1} + f_n\right] - \frac{h^4(b-a)}{180} f^{(4)}(\xi)$$

Change of Variables Formula and Infinite Domains

- Problem: How do we approximate integrals with infinite domains?

$$\int_0^{\infty} f(x)dx \equiv \lim_{b\to\infty} \int_0^{b} f(x)dx$$

- Truncation (a bad idea): For large b, use

$$\int_0^{\infty} f(x)dx \doteq \int_0^{b} f(x)dx$$

- Change of variables theorem:
  Theorem 1 If $\phi : \mathbb{R} \to \mathbb{R}$ is a monotonically increasing, C^1 function on the (possibly infinite) interval $[a, b]$, then for any integrable $g(x)$ on $[a, b]$,

$$\int_a^b g(y)dy = \int_{\phi^{-1}(a)}^{\phi^{-1}(b)} g(\phi(x))\phi'(x)dx$$

Change of Variables Formula and Infinite Domains

- COV Objective: find a $x(z)$ function such that

$$\int_0^\infty f(x)dx = \int_0^1 f(x(z))x'(z)dz$$

can be accurately computed

  - $x : (0, \infty) \to (0, 1) : \quad x(z) = \frac{z}{1-z}, x'(z) = \frac{1}{(1-z)^2}$
    - Example:

$$\int_0^\infty e^{-t} t^n dt = \int_0^1 e^{-z/(1-z)} \left(\frac{z}{1-z} \right)^n (1-z)^{-2} dz$$

    - All derivatives are bounded, so Newton-Cotes error bound formulas applies.

Change of Variables Formula and Infinite Domains

- $x : (-\infty, \infty) \to (0, 1) : \quad x(z) = \ln\left(\frac{z}{1-z}\right), x'(z) = (z(1-z))^{-1}$
  - Example: $\int_{-\infty}^{\infty} e^{-x^2} f(x)dx$ becomes

$$\begin{aligned} &\int_0^1 e^{-\left(\ln \frac{z}{(1-z)}\right)^2} f\left(\ln\left(\frac{z}{1-z}\right)\right) \frac{dz}{(1-z)z} \\ = &\int_0^1 \left(\frac{1-z}{z}\right)^{\ln \frac{z}{(1-z)}} f\left(\ln\left(\frac{z}{1-z}\right)\right) \frac{dz}{z(1-z)} \end{aligned}$$

  - Integrand's derivatives are bounded if f is exponentially bounded
- Bad COV formula
  - $x(z) = \left(\ln \frac{z}{1-z}\right)^{1/3}$ maps (0, 1) onto $(-\infty, \infty)$
  - Application to $\int_{-\infty}^{\infty} e^{-x^2} f(x)dx$ often results in integrand with unbounded derivatives.

Gaussian Formulas

- All integration formulas are of form

$$\int_a^b f(x)dx \doteq \sum_{i=1}^{n} \omega_i f(x_i)$$

for some quadrature nodes $x_i \in [a, b]$ and quadrature weights ω_i.

  - Newton-Cotes use arbitrary x_i
  - Gaussian quadrature uses good choices of x_i nodes and ω_i weights.

Gauss-Chebyshev Quadrature

- Domain: [-1, 1]
- Weight: $(1 - x^2)^{(-1/2)}$
- Formula:

$$\int_{-1}^{1} f(x)\left(1 - x^2\right)^{-1/2} dx = \frac{\pi}{n} \sum_{i=1}^{n} f\left(x_i\right) + \frac{\pi}{2^{2n-1}} \frac{f^{(2n)}(\xi)}{(2n)!}$$

for some $\xi \in [-1, 1]$, with quadrature nodes

$$x_i = \cos\left(\frac{2i-1}{2n}\pi\right), \quad i = 1, \ldots, n$$

Arbitrary Domains

- Want to approximate $\int_a^b f(y)dy$
  - Different range, no weight function
  - Linear change of variables $x = -1 + 2(y-a)(b-a)$
  - Multiply the integrand by $\left(1-x^2\right)^{1/2} / \left(1-x^2\right)^{1/2}$.
  - C.O.V. formula

$$\int_a^b f(y)dy = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{(x+1)(b-a)}{2}+a\right)\frac{\left(1-x^2\right)^{1/2}}{\left(1-x^2\right)^{1/2}}dx$$

  - Gauss-Chebyshev quadrature produces

$$\int_a^b f(y)dy \doteq \frac{\pi(b-a)}{2n}\sum_{i-1}^{n} f\left(\frac{(x_i+1)(b-a)}{2}+a\right)\left(1-x_i^2\right)^{1/2}$$

where the x_i are Gauss-Chebyshev nodes over [-1, 1].

Gauss-Legendre Quadrature

- Domain: [-1, 1]
- Weight: 1
- Formula:

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} \omega_i f\left(x_i\right) + \frac{2^{2n+1}(n!)^4}{(2n+1)!(2n)!} \cdot \frac{f^{(2n)}(\xi)}{(2n)!}$$

  for some $-1 \leq \xi \leq 1$.
- In general,

$$\int_{a}^{b} f(x)dx \doteq \frac{b-a}{2} \sum_{i=1}^{n} \omega_i f\left(\frac{\left(x_i+1\right)(b-a)}{2} + a\right)$$

Gauss - Legendre Quadrature

N	x_i	ω_i
2	0.5773502691	0.1000000000(1)
3	0.7745966692	0.5555555555
	0.0000000000	0.8888888888
5	0.9061798459	0.2369268850
	0.5384693101	0.4786286704
	0.0000000000	0.5688888888
10	0.9739065285	0.6667134430(−1)
	0.8650633666	0.1494513491
	0.6794095682	0.2190863625
	0.4333953941	0.2692667193
	0.1488743389	0.2955242247

Exercise

Compute $\int_a^b f(x)dx$, where $a = 0, b = 1, f(x) = x^2 - 2x + 1$

- Use Midpoint rule (set $n = 5$)
- Use Gauss-Legendre Quadrature (use GLeg 5)

Life-cycle example:

- $c(t) = 1 + t/5 - 7(t/50)^2$, where $0 \leq t \leq 50$.
- Discounted utility is $\int_0^{50} e^{-\rho t} u(c(t)) dt$
- $\rho = 0.05,\ u(c) = c^{1+\gamma}/(1+\gamma)$.
- Errors in computing $\int_0^{50} \frac{e^{-.05t}}{1+\gamma} \left(1 + \frac{t}{5} - 7\left(\frac{t}{50}\right)^2\right)^{1+\gamma} dt$

	$\gamma =$	.5	1.1	3	10
Truth		1.24431	.664537	.149431	.0246177
Rule:	GLeg 3	5(−3)	2(−3)	3(−2)	2(−2)
	GLeg 5	1(−4)	8(−5)	5(−3)	2(−2)
	GLeg 10	1(−7)	1(−7)	2(−5)	2(−3)
	GLeg 15	1(−10)	2(−10)	9(−8)	4(−5)
	GLeg 20	7(−13)	9(−13)	3(−10)	6(−7)

Gauss-Hermite Quadrature

- Domain: $[-\infty, \infty]$
- Weight: e^{-x^2}
- Formula:

$$\int_{-\infty}^{\infty} f(x)e^{-x^2}dx = \sum_{i=1}^{n} \omega_i f(x_i) + \frac{n!\sqrt{\pi}}{2^n} \cdot \frac{f^{(2n)}(\xi)}{(2n)!}$$

for some $\xi \in (-\infty, \infty)$.

Gauss - Hermite Quadrature

N	x_i	ω_i
2	0.7071067811	0.8862269254
3	0.1224744871(1)	0.2954089751
	0.0000000000	0.1181635900(1)
4	0.1650680123(1)	0.8131283544(−1)
	0.5246476232	0.8049140900
7	0.2651961356(1)	0.9717812450(−3)
	0.1673551628(1)	0.5451558281(−1)
	0.8162878828	0.4256072526
	0.0000000000	0.8102646175
10	0.3436159118(1)	0.7640432855(−5)
	0.2532731674(1)	0.1343645746(−2)
	0.1756683649(1)	0.3387439445(−1)
	0.1036610829(1)	0.2401386110
	0.3429013272	0.6108626337

Normal Random Variables

- Y is distributed $N\left(\mu, \sigma^2\right)$
- Expectation is integration:

$$E\{f(Y)\} = \left(2\pi\sigma^2\right)^{-1/2} \int_{-\infty}^{\infty} f(y) e^{-\frac{(y-\mu)^2}{2\sigma^2}}\, dy$$

- Use Gauss-Hermite quadrature
  - linear COV: $x = (y-\mu)/\sqrt{2}\sigma$
  - COV formula:

$$\int_{-\infty}^{\infty} f(y) e^{-(y-\mu)^2/\left(2\sigma^2\right)} dy = \int_{-\infty}^{\infty} f(\sqrt{2}\sigma x + \mu) e^{-x^2} \sqrt{2}\sigma\, dx$$

  - COV quadrature formula:

$$E\{f(Y)\} \doteq \pi^{-\frac{1}{2}} \sum_{i=1}^{n} \omega_i f\left(\sqrt{2}\sigma x_i + \mu\right)$$

  where the ω_i and x_i are the Gauss-Hermite quadrature weights and nodes over $[-\infty, \infty]$.

- Portfolio example
  - An investor holds one bond which will be worth 1 in the future and equity whose value is Z, where $\ln Z \sim \mathcal{N}\left(\mu, \sigma^2\right)$.
  - Expected utility is

$$U = \left(2\pi\sigma^2\right)^{-1/2} \int_{-\infty}^{\infty} u\left(1 + e^z\right) e^{-(z-\mu)^2/2\sigma^2} dz$$

$$u(c) = \frac{c^{1+\gamma}}{1+\gamma}$$

  and the certainty equivalent is $u^{-1}(U)$.
  - Errors in certainty equivalents

Rule	γ :	$-.5$	-1.1	-2.0	-5.0	-10.0
GH2		$1(-4)$	$2(-4)$	$3(-4)$	$6(-3)$	$3(-2)$
GH3		$1(-6)$	$3(-6)$	$9(-7)$	$7(-5)$	$9(-5)$
GH4		$2(-8)$	$7(-8)$	$4(-7)$	$7(-6)$	$1(-4)$
GH7		$3(-10)$	$2(-10)$	$3(-11)$	$3(-9)$	$1(-9)$
GH13		$3(-10)$	$2(-10)$	$3(-11)$	$5(-14)$	$2(-13)$

Gauss-Laguerre Quadrature

- Domain: $[0, \infty]$
- Weight: e^{-x}
- Formula:

$$\int_0^\infty f(x)e^{-x}dx = \sum_{i=1}^{n} \omega_i f(x_i) + (n!)^2 \frac{f^{(2n)}(\xi)}{(2n)!}$$

for some $\xi \in [0, \infty)$.

- General integral
  - Linear COV $x = r(y - a)$
  - COV formula

$$\int_a^\infty e^{-ry} f(y)dy \doteq \frac{e^{-ra}}{r} \sum_{i=1}^{n} \omega_i f\left(\frac{x_i}{r} + a\right)$$

where the ω_i and x_i are the Gauss-Laguerre quadrature weights and nodes over $[0, \infty]$.

Gauss-Laguerre Quadrature

N	x_i	ω_i
2	0.5857864376	0.8535533905
	0.3414213562(1)	0.1464466094
3	0.4157745567	0.7110930099
	0.2294280360(1)	0.2785177335
	0.6289945082(1)	0.1038925650(−1)
4	0.3225476896	0.6031541043
	0.1745761101(1)	0.3574186924
	0.4536620296(1)	0.3888790851(−1)
	0.9395070912(1)	0.5392947055(−3)
7	0.1930436765	0.4093189517
	0.1026664895(1)	0.4218312778
	0.2567876744(1)	0.1471263486
	0.4900353084(1)	0.2063351446(−1)
	0.8182153444(1)	0.1074010143(−2)
	0.1273418029(2)	0.1586546434(−4)
	0.1939572786(2)	0.3170315478(−7)

- Present Value Example
  - Use Gauss-Legendre quadrature to compute present values.
  - Suppose discounted profits equal

$$\int_0^{\infty} e^{-rt} m(t)^{1-\lambda} dt$$

  - Errors:

		$r = .05$	$r = .10$	$r = .05$
		$\lambda = .05$	$\lambda = .05$	$\lambda = .20$
Truth:		49.7472	20.3923	74.4005
Errors:	GLag 4	$3(-1)$	$4(-2)$	$6(0)$
	GLag 5	$7(-3)$	$7(-4)$	$3(0)$
	GLag 10	$3(-3)$	$6(-5)$	$2(-1)$
	GLag 15	$6(-5)$	$3(-7)$	$6(-2)$
	GLag 20	$3(-6)$	$8(-9)$	$1(-2)$

General Applicability of Gaussian Quadrature

Comparisons with Newton-Cotes formulas

Rule	n	$\int_0^1 x^{1/4} dx$	$\int_1^{10} x^{-2} dx$	$\int_0^1 e^x dx$	$\int_1^{-1} (x+.05)^+ dx$
Trapezoid	4	0.7212	1.7637	1.7342	0.6056
	7	0.7664	1.1922	1.7223	0.5583
	10	0.7797	1.0448	1.7200	0.5562
	13	0.7858	0.9857	1.7193	0.5542
Simpson	3	0.6496	1.3008	1.4662	0.4037
	7	0.7816	1.0017	1.7183	0.5426
	11	0.7524	0.9338	1.6232	0.4844
	15	0.7922	0.9169	1.7183	0.5528
G-Legendre	4	0.8023	0.8563	1.7183	0.5713
	7	0.8006	0.8985	1.7183	0.5457
	10	0.8003	0.9000	1.7183	0.5538
	13	0.8001	0.9000	1.7183	0.5513
Truth		.80000	.90000	1.7183	0.55125

Multidimensional Integration

- Most economic problems have several dimensions
  - Multiple assets
  - Multiple error terms
- Multidimensional integrals are much more difficult
  - Simple methods suffer from curse of dimensionality
  - There are methods which avoid curse of dimensionality

Product Rules

- Build product rules from one-dimension rules
- Let $x_i^\ell, \omega_i^\ell, \quad i = 1, \cdots, m$, be one-dimensional quadrature points and weights in dimension ℓ from a Newton-Cotes rule or the Gauss-Legendre rule.
- The *product rule*

$$\int_{[-1,1]^d} f(x)dx \doteq \sum_{i_1=1}^{m} \cdots \sum_{i_d=1}^{m} \omega_{i_1}^1 \omega_{i_2}^2 \cdots \omega_{i_d}^d f\left(x_{i_1}^1, x_{i_2}^2, \cdots, x_{i_d}^d\right)$$

Product Rules

- Gaussian structure prevails
  - Suppose $w^{\ell}(x)$ is weighting function in dimension ℓ
  - Define the d-dimensional weighting function.

$$W(x) \equiv W\left(x_1, \cdots, x_d\right) = \prod_{\ell-1}^{d} w^{\ell}\left(x_{\ell}\right)$$

  - Product Gaussian rules are based on product orthogonal polynomials.
- Curse of dimensionality:
  - m^d functional evaluations is m^d for a d-dimensional problem with m points in each direction.
  - Problem worse for Newton-Cotes rules which are less accurate in $\mathbb{R}^1$.
  - Monte-Carlo simulations may be a better way to calculate the integration when we have high-dimensional problems.