Numerical Methods in Economics

MIT Press, 1998

Notes for Chapter 7: Numerical Integration and Differentiation

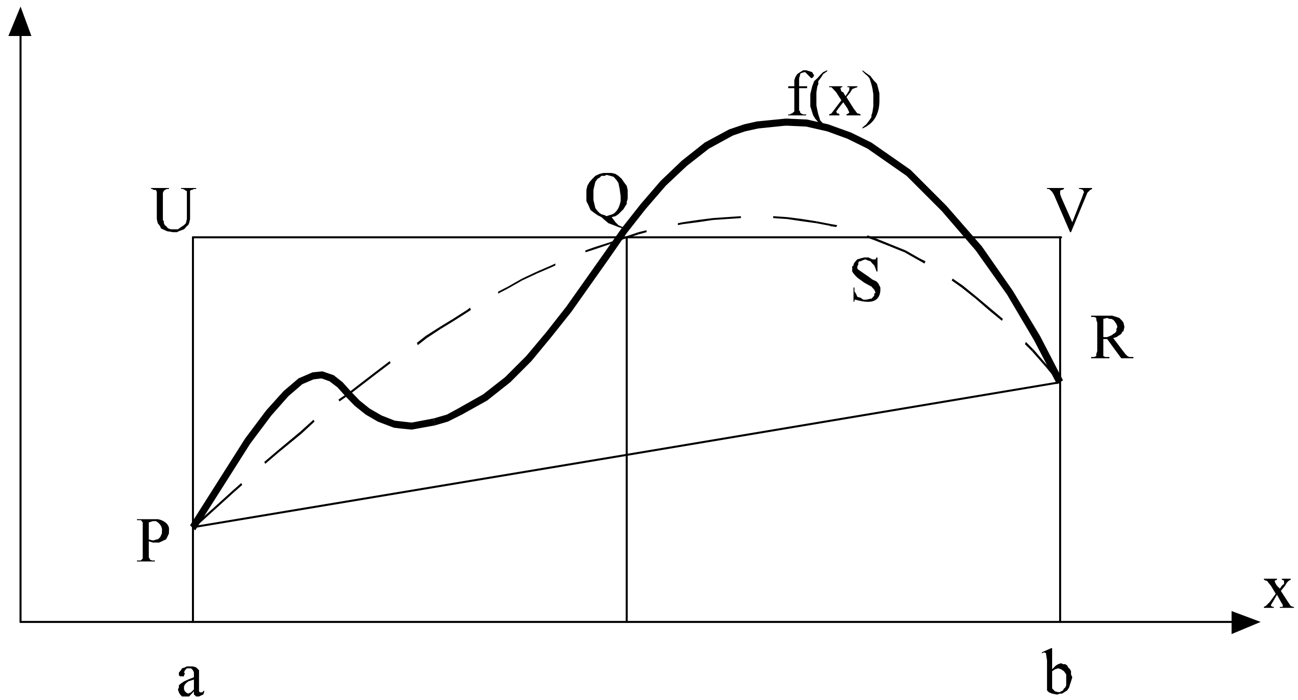
November 22, 2006

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



- 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 interpolating $f(x)$ at a and b
  - Integral approximation is trapezoid $aPRb$

- Parabolic function approximation:
  - Compute parabola interpolating $f(x)$ at a, b, and $(a+b)/2$
  - Integral approximation is area of $aPQRb$

- Midpoint Rule: piecewise step function approximation

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

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

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

- 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 $\xi \in [a,\, b]$

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

- 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 $\xi \in [a, b]$

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

- Obscure rules for degree 3, 4, etc. approximations.

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 $g(y)$ on $[a, b]$,*

$$\int_a^b g(y)\ dy = \int_{\phi^{-1}(a)}^{\phi^{-1}(b)} g(\phi(x))\ \phi'(x)\ dx. \tag{7.1.8}$$

- 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.

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

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

    * 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 $\int_{-\infty}^{\infty} f(x) e^{-x^2}\, dx$ often creates an integrand with unbounded derivatives.

Gaussian Formulas

- All integration formulas are of form

$$\int_a^b f(x)\,dx \doteq \sum_{i=1}^{n} \omega_i f(x_i) \tag{7.2.1}$$

  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.

- Exact quadrature formulas:

  – Let $\mathcal{F}_k$ be the space of degree k polynomials

  – A quadrature formula is exact of degree k if it correctly integrates each function in $\mathcal{F}_k$

  – Gaussian quadrature formulas use n points and are exact of degree $2n-1$

Theorem 2 *Suppose that* $\{\varphi_k(x)\}_{k=0}^{\infty}$ *is an orthonormal family of polynomials with respect to* $w(x)$ *on* $[a,\, b]$*.*

1. *Define* q_k *so that* $\varphi_k(x) = q_k\, x^k + \cdots$ *.*

2. *Let* x_i*,* $i = 1, ..., n$ *be the* n *zeros of* $\varphi_n(x)$

3. *Let* $\omega_i = \; - \frac{q_{n+1}/q_n}{\varphi_n'(x_i)\, \varphi_{n+1}\,(x_i)} > 0$

Then

1. $a < x_1 < x_2 < \cdots < x_n < b$*;*

2. *if* $f \in C^{(2n)}[a,\, b]$*, then for some* $\xi \in [a,\, b]$*,*

$$\int_a^b w(x)\, f(x)\; dx = \sum_{i=1}^{n} \omega_i\, f(x_i) + \frac{f^{(2n)}(\xi)}{q_n^2 (2n)!};$$

3. *and* $\sum_{i=1}^{n} \omega_i f(x_i)$ *is the unique formula on* n *nodes that exactly integrates* $\int_a^b f(x)\, w(x)\, dx$ *for all polynomials in* $\mathcal{F}_{2n-1}$*.*

Gauss-Chebyshev Quadrature

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

$$\int_{-1}^{1} f(x)(1 - x^2)^{-1/2}\, dx = \frac{\pi}{n} \sum_{i=1}^{n} f(x_i) + \frac{\pi}{2^{2n-1}} \frac{f^{(2n)}(\xi)}{(2n)!} \tag{7.2.4}$$

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

$$x_i = cos\left(\frac{2i-1}{2n}\pi\right), \quad i = 1, ..., n. \tag{7.2.5}$$

Arbitrary Domains

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

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

  - 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:

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

  for some $-1 \leq \xi \leq 1$.

- Convergence:
  - use $n! \doteq e^{-n-1}\, n^{n+1/2}\, \sqrt{2\pi n}$
  - error bounded above by $\pi 4^{-n}\, M$

$$M = \sup_{m} \left[\max_{-1 \leq x \leq 1} \frac{f^{(m)}(x)}{m!} \right]$$

  - Exponential convergence for analytic functions

- In general,

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

- Use values for Gaussian nodes and weights from tables instead of programs; tables will have 16 digit accuracy

Table 7.2: 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

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 $\int_0^{50} e^{-.05t} \left(1 + \frac{t}{5} - 7\left(\frac{t}{50}\right)^2\right)^{1-\gamma} dt$

	$\gamma=$	.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 $\xi \in (-\infty, \infty)$.

Table 7.4: 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 $N(\mu, \sigma^2)$
  - Expectation is integration:

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

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

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

    * COV quadrature formula:

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

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 $\ln Z \sim \mathcal{N}(\mu, \sigma^2)$.

  – Expected utility is

$$U = (2\pi\sigma^2)^{-1/2} \int_{-\infty}^{\infty} u(1+e^z) e^{-(z-\mu)^2/2\sigma^2}\, dz \qquad (7.2.12)$$

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

  and the certainty equivalent of (7.2.12) is $u^{-1}(U)$.

  – Errors in certainty equivalents: Table 7.5

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)

- The certainty equivalent of (7.2.12) with $\mu = 0.15$ and $\sigma = 0.25$ is 2.34. So, relative errors are roughly the same.

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 $[0, \infty]$.

Table 7.6: 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-Laguerre quadrature to compute present values.
  - Suppose discounted profits equal

$$\eta\left(\frac{\eta-1}{\eta}\right)^{\eta-1}\int_0^\infty e^{-rt}m(t)^{1-\eta}\,dt.$$

  - Errors: Table 7.7

		$r=.05$	$r=.10$	$r=.05$
		$\lambda=.05$	$\lambda=.05$	$\lambda=.20$
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)

  - Gauss-Laguerre integration implicitly assumes that $m(t)^{1-\eta}$ is a polynomial.
    - ∗ When $\lambda = 0.05$, $m(t)$ is nearly constant
    - ∗ When $\lambda = 0.20$, $m(t)^{1-\eta}$ is less polynomial-like.

General Applicability of Gaussian Quadrature

Theorem 3 *(Gaussian quadrature convergence) If f is Riemann Integrable on $[a, b]$, the error in the n-point Gauss-Legendre rule applied to $\int_a^b f(x)\,dx$ goes to 0 as $n \to \infty$.*

Comparisons with Newton-Cotes formulas: Table 7.1

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*

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

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

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

  - 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 $\mathbb{R}^1$.

Monomial Formulas: A Nonproduct Approach

- Method
- Choose $x^i \in D \subset \mathbb{R}^d,\ i = 1, ..., N$
- Choose $\omega_i \in \mathbb{R},\ i = 1, ..., N$
- Quadrature formula

$$\int_D f(x)\,dx \doteq \sum_{i=1}^{N} \omega_i\, f(x^i) \tag{7.5.3}$$

- A monomial formula is complete for degree ℓ if

$$\sum_{i=1}^{N} \omega_i\, p(x^i) = \int_D p(x)\,dx \tag{7.5.3}$$

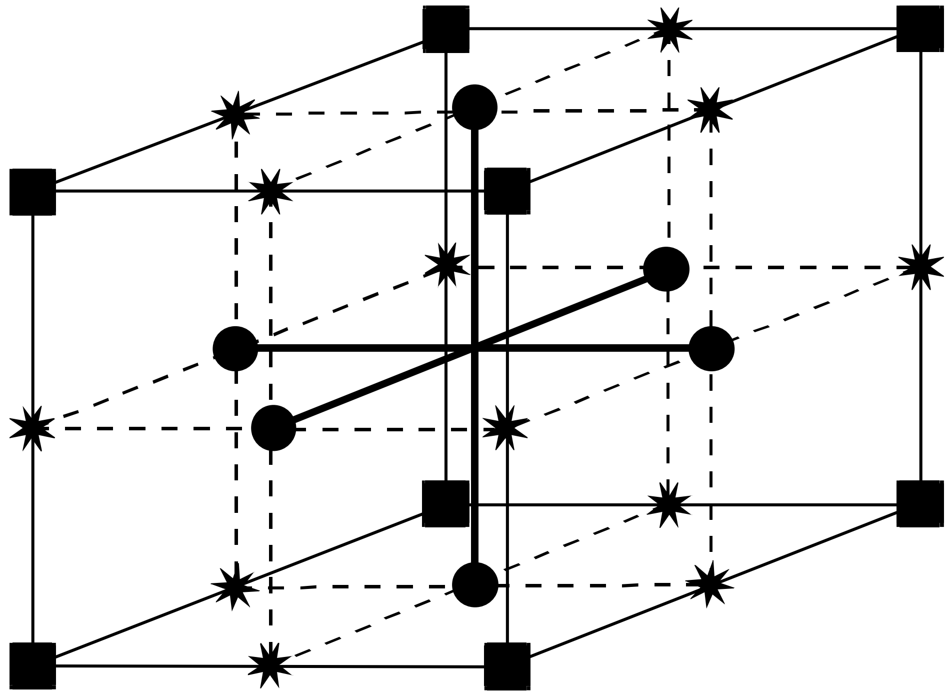
  for all polynomials $p(x)$ of total degree ℓ; recall that $\mathcal{P}_\ell$ was defined in chapter 6 to be the set of such polynomials.

- For the case $\ell = 2$, this implies the equations

$$\begin{aligned} \textstyle\sum_{i=1}^{N} \omega_i &= \textstyle\int_D 1 \cdot dx \\ \textstyle\sum_{i=1}^{N} \omega_i x_j^i &= \textstyle\int_D x_j\,dx,\ j = 1, \cdots, d \\ \textstyle\sum_{i=1}^{N} \omega_i x_j^i x_k^i &= \textstyle\int_D x_j x_k\,dx,\ j, k = 1, \cdots, d \end{aligned} \tag{7.5.4}$$

  - $1 + d + \frac{1}{2}d(d+1)$ equations
  - N weights ω_i and the N nodes x^i each with d components, yielding a total of $(d+1)N$ unknowns.

Quadrature Node Sets



- Natural types of nodes:
  - The center
  - The circles: centers of faces
  - The stars: centers of edges
  - The squares: vertices

- Some monomial formulas will take some combinations of these sets
- Other types of collections are possible

- Simple examples
  - Let $e^j \equiv (0, \ldots, 1, \ldots, 0)$ where the '1' appears in column j.
  - $2d$ points and exactly integrates all elements of $\mathcal{P}_3$ over $[-1,1]^d$

$$\int_{[-1,1]^d} f \doteq \omega \sum_{i=1}^{d} \left(f(ue^i) + f(-ue^i) \right)$$

$$u = \left(\frac{d}{3}\right)^{1/2}, \quad \omega = \frac{2^{d-1}}{d}$$

  - For $\mathcal{P}_5$ the following scheme works:

$$\begin{aligned}\int_{[-1,1]^d} f \doteq & \omega_1 f(0) + \omega_2 \sum_{i=1}^{d} \left(f(ue^i) + f(-ue^i) \right) \\ & + \omega_3 \sum_{\substack{1 \le i < d, \\ i < j \le d}} \left(f(u(e^i \pm e^j)) + f(-u(e^i \pm e^j)) \right)\end{aligned}$$

  where

$$\begin{aligned}\omega_1 &= 2^d(25\, d^2 - 115\, d + 162), \quad \omega_2 = 2^d(70 - 25d) \\ \omega_3 &= \frac{25}{324}\, 2^d, \quad u = (\frac{3}{5})^{1/2}.\end{aligned}$$

- Smolyak (a.k.a., sparse) grids (see pictures on next slide)

Existence Result for Monomial Formulas

Theorem 4 *(Mysovskikh) Let $w(x)$ be a nonnegative weighting function on $D \subset \mathbb{R}^d$ such that each moment*

$$\int_D w(x) x_1^{i_1} \cdots x_d^{i_d} \, dx_1 \cdots dx_d$$

exists for $i_1, \cdots, i_d \geq 0$, $i_1 + \cdots + i_d \leq m$. Then, for some $N \leq (m+d)!/(m!d!)$, there exists N positive weights, ω_i, and N nodes, x^i, such that for each multi-index $|\alpha| \leq m$,

$$\int_D w(x) x^\alpha \, dx = \sum_{i=1}^{N} \omega_i (x^i)^\alpha .$$

- Purely existential
- Solving equations is difficult
- Formulas do not suffer from curse of dimensionality
- See Stroud and Secrest book for a large list of formulas.

Numerical Differentiation

- One-sided formula

$$f'(x) \doteq \frac{f(x+h) - f(x)}{h} \tag{7.7.1}$$

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

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

  - Error bound is

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

  - 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, then error bound is

$$\mid f'(x) - D(h) \mid \leq \frac{2\varepsilon}{h} + \frac{h}{2} M_2 \tag{7.7.2}$$

  - Upper bound on error is minimized at

$$h^* = 2\sqrt{\frac{\varepsilon}{M_2}} \tag{7.7.3}$$

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

- Two-Sided Difference Formula
  - Two-sided formula
$$f'(x) \doteq \frac{f(x+h) - f(x-h)}{2h} \tag{7.7.4}$$
  - 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 $\varepsilon^{2/3}$.
  - On a twelve-digit machine: eight-digit accuracy versus six-digit accuracy.
- General Problem
  - Find n-point difference approximation for $f^{(k)}(x)$
  - Optimal step size can be determined by Taylor-series expansions and linear equations.