

Numerical Differentiation and Integration

Zi Wang
HKBU

Spring 2025

Numerical Differentiation

- Forward differencing:

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

- $\frac{\partial f(x)}{\partial x_i} \simeq \frac{f(x_1, \dots, x_i + h_i, \dots, x_n) - f(x_1, \dots, x_i, \dots, x_n)}{h_i}$

- Backward differencing:

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

- $\frac{\partial f(x)}{\partial x_i} \simeq \frac{f(x_1, \dots, x_i, \dots, x_n) - f(x_1, \dots, x_i - h_i, \dots, x_n)}{h_i}$

- Note:

- In practice, one uses forward or backward differences depending on whether we care more about left or right derivative

- $h = \max(|x|, 1) \sqrt{\epsilon}$ where ϵ is the machine precision (about 10^{-15} in the Matlab)

Numerical Differentiation

- Centered differencing:

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

- $\frac{\partial f(x)}{\partial x_i} \simeq \frac{f(x_1, \dots, x_i+h_i, \dots, x_n) - f(x_1, \dots, x_i-h_i, \dots, x_n)}{2h_i}$

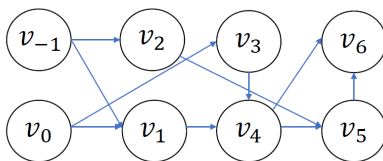
- Richardson's extrapolation (a fourth-order approximation):

$$f'(x) \simeq \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} \quad (1)$$

- Example: $y = f(x_1, x_2) = [x_1^2 + x_1/x_2 - \exp(x_2)] [x_1/x_2 - \exp(x_2)]$ at $(1, 1)$

Automatic Differentiation

- Example: $y = [x_1^2 + x_1/x_2 - \exp(x_2)] [x_1/x_2 - \exp(x_2)]$
 - Intermediate variables: $v_{-1} = x_1$, $v_0 = x_2$, $v_1 = v_{-1}/v_0$, $v_2 = v_{-1}^2$, $v_3 = \exp(v_0)$, $v_4 = v_1 - v_3$, $v_5 = v_2 + v_4$, and $v_6 = v_4 \cdot v_5 = y$
 - Computational graph:



- By the chain rule

$$\frac{\partial y}{\partial x_1} = \frac{\partial y}{\partial v_6} \left(\frac{\partial v_6}{\partial v_4} \frac{\partial v_4}{\partial v_1} \frac{\partial v_1}{\partial v_{-1}} + \frac{\partial v_6}{\partial v_5} \left(\frac{\partial v_5}{\partial v_4} \frac{\partial v_4}{\partial v_1} \frac{\partial v_1}{\partial v_{-1}} + \frac{\partial v_5}{\partial v_2} \frac{\partial v_2}{\partial v_{-1}} \right) \right) \frac{\partial v_{-1}}{\partial x_1} \quad (2)$$

$$\frac{\partial y}{\partial x_2} = \frac{\partial y}{\partial v_6} \left(\frac{\partial v_6}{\partial v_4} \left(\frac{\partial v_4}{\partial v_1} \frac{\partial v_1}{\partial v_0} + \frac{\partial v_4}{\partial v_3} \frac{\partial v_3}{\partial v_0} \right) + \frac{\partial v_6}{\partial v_5} \frac{\partial v_5}{\partial v_4} \frac{\partial v_4}{\partial v_1} \frac{\partial v_1}{\partial v_0} \right) \frac{\partial v_0}{\partial x_2}$$

Numerical Quadrature Methods

- Integration:

$$S = \int_I f(x) dx \quad (3)$$

- Quadrature:

$$\int_I f(x) dx \simeq \sum_{i=1}^n w_i f(x_i) \quad (4)$$

- Quadrature methods differ only in how the quadrature weights w_i and the quadrature nodes x_i are chosen

Newton-Cotes Methods

- Integration:

$$\int_a^b f(x) dx \quad (5)$$

- Trapezoid rule:

- $x_i = a + (i - 1) h$ where $h = (b - a) / n$
- $\int_a^b f(x) dx \simeq \sum_{i=1}^n w_i f(x_i)$ where $w_1 = w_n = h/2$ and $w_i = h$, otherwise

- Simpson's rule: piece-wise quadratic

- $x_i = a + (i - 1) h$ where $h = (b - a) / (n - 1)$ and n is odd
- $\int_{x_{2j-1}}^{x_{2j+1}} f(x) dx \simeq \frac{h}{3} [f(x_{2j-1}) + 4f(x_{2j}) + f(x_{2j+1})]$
- $\int_a^b f(x) dx \simeq \sum_{i=1}^n w_i f(x_i)$ where $w_1 = w_n = h/3$ and, otherwise, $w_i = 4h/3$ if i is odd and $w_i = 2h/3$ if i is even

Newton-Cotes Methods: Higher dimensional Integration

- Integration:

$$\int_{x_1 \in [a_1, b_1]} \int_{x_2 \in [a_2, b_2]} f(x_1, x_2) dx_1 dx_2 \quad (6)$$

- Newton-Cotes nodes and weights:

- $\{(x_{1i}, w_{1i}) \mid i = 1, 2, \dots, n_1\}$
- $\{(x_{2j}, w_{2j}) \mid j = 1, 2, \dots, n_2\}$
- Nodes: $\{(x_{1i}, x_{2j}) \mid i = 1, 2, \dots, n_1; j = 1, 2, \dots, n_2\}$
- Weights: $\{w_{ij} = w_{1i} w_{2j} \mid i = 1, 2, \dots, n_1; j = 1, 2, \dots, n_2\}$

Gaussian Quadrature

- Integration:

$$\int_{-1}^1 f(x) dx = \sum_{i=1}^n w_i f(x_i) \quad (7)$$

- Nodes: x_i are the roots of a Legendre polynomial of degree n , $P_n(x)$

- Weights: $w_i = \frac{2}{(1-x_i^2)[P'_n(x_i)]^2}$

- Legendre polynomials:

- Generating function: $\frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(t)t^n$, where $P_0(x) = 1$ and $P_1(x) = x$

- Recursive: $(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$

- Rodrigues' formula: $P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n$

Monte Carlo Integration

- Integration (multi-dimensional): $S = \int_I f(x) dx$
- Let $V = \int_I dx$
- n uniform samples: $x_1, \dots, x_n \in I$
- Then $S \simeq \frac{V}{n} \sum_{i=1}^n f(x_i)$

Numerical Integration: Example

- $H(x, y) = \begin{cases} 1 & \text{if } x^2 + y^2 \leq 1 \\ 0 & \text{else} \end{cases}$
- Let $I = [-1, 1] \times [-1, 1]$. Compute

$$S = \int_I H(x, y) dx dy \quad (8)$$

Example: Variable Markups in the Quantitative Trade Model

- $i = 1, \dots, N$ countries with labor $(L_i)_{i=1}^N$
- The *Kimball's* preference over a continuum of varieties:

$$\int_{\omega \in \Omega_n} H\left(\frac{q_n(\omega)}{Q_n}\right) d\omega = 1, \quad (9)$$

where Q_n is the aggregate consumption and the function $H(\cdot)$ is strictly increasing, strictly concave, and satisfies $H(1) = 1$

- CES as a special case: $H(q) = q^{\frac{\sigma-1}{\sigma}}$ for $\sigma > 1$

Example: Variable Markups in the Quantitative Trade Model

- The inverse demand function of variety ω in country n can be expressed as

$$\frac{p_n(\omega)}{P_n} = H' \left(\frac{q_n(\omega)}{Q_n} \right) D_n, \quad (10)$$

where the *demand index*

$$D_n = \left[\int_{\omega \in \Omega_n} H' \left(\frac{q_n(\omega)}{Q_n} \right) \frac{q_n(\omega)}{Q_n} d\omega \right]^{-1}, \quad (11)$$

and the price index for final goods

$$P_n = \int_{\omega \in \Omega_n} p_n(\omega) \frac{q_n(\omega)}{Q_n} d\omega = \int_{\omega \in \Omega_n} p_n(\omega) H'^{-1} \left(\frac{p_n(\omega)}{P_n} \frac{1}{D_n} \right) d\omega \quad (12)$$

Example: Variable Markups in the Quantitative Trade Model

- Klenow and Willis (2016):

$$H(q) = 1 + (\sigma - 1) \exp\left(\frac{1}{\varepsilon}\right) \varepsilon^{\frac{\sigma}{\varepsilon}-1} \left[\Gamma\left(\frac{\sigma}{\varepsilon}, \frac{1}{\varepsilon}\right) - \Gamma\left(\frac{\sigma}{\varepsilon}, \frac{q^{\frac{\varepsilon}{\sigma}}}{\varepsilon}\right) \right], \quad (13)$$

with $\sigma > 1$ and $\varepsilon \geq 0$ and where $\Gamma(s, x)$ denotes the upper incomplete Gamma function

$$\Gamma(s, x) := \int_x^\infty t^{s-1} e^{-t} dt \quad (14)$$

- $\varepsilon = 0$: the CES case $H(q) = q^{\frac{\sigma-1}{\sigma}}$
- We have

$$H'(q) = \frac{\sigma - 1}{\sigma} \exp\left(\frac{1 - q^{\frac{\varepsilon}{\sigma}}}{\varepsilon}\right) \quad (15)$$

Example: Variable Markups in the Quantitative Trade Model

- Each variety ω is produced by a firm using labor under monopolistic competition
- Fixed marketing cost of firms to serve market n : F_n in units of n 's production labor
- Iceberg trade cost from country ℓ to n : $\tau_{\ell n} \geq 1$ with $\tau_{\ell \ell} = 1$
- After paying a fixed entry cost f^e in terms of country i 's labor, firm ω draws a productivity $\varphi_i(\omega)$ from

$$\Pr(\varphi_i(\omega) \leq \varphi) = 1 - T_i \varphi^{-\theta}, \quad (16)$$

with support $\varphi \geq T_i^{\frac{1}{\theta}}$

Example: Variable Markups in the Quantitative Trade Model

- Conditional on firm ω from country i serving country n , its effective cost $c_{in}(\omega) = \frac{w_i \tau_{in}}{\varphi_i(\omega)}$ satisfies

$$\Pr(c_{in}(\omega) \leq c) = \bar{T}_{in}^\theta c^\theta, \quad c \leq \frac{1}{\bar{T}_{in}}, \quad \bar{T}_{in} \equiv T_i^{\frac{1}{\theta}} (w_i \tau_{in})^{-1} \quad (17)$$

- The operating profit of firm ω from country i serving market n is

$$\tilde{\pi}_{in}(\omega) = \max_{q_{in}(\omega) \geq 0} \left[H' \left(\frac{q_{in}(\omega)}{Q_n} \right) D_n P_n - c_{in}(\omega) \right] q_{in}(\omega). \quad (18)$$

- Let $s_{in}(\omega) := \frac{q_{in}(\omega)}{Q_n}$ be the relative output. The optimal price can be expressed as a markup over the unit cost:

$$p_{in}(\omega) = \mu(s_{in}(\omega)) c_{in}(\omega), \quad \mu(s_{in}(\omega)) := \frac{\sigma s_{in}(\omega)^{-\frac{\varepsilon}{\sigma}}}{\sigma s_{in}(\omega)^{-\frac{\varepsilon}{\sigma}} - 1}. \quad (19)$$

- Let $X_n := P_n Q_n$. Then the operating profit can be expressed as

$$\tilde{\pi}_{in}(\omega) = \frac{s_{in}(\omega)^{\frac{\varepsilon}{\sigma}}}{\sigma} \frac{\sigma - 1}{\sigma} \exp \left(\frac{1 - s_{in}(\omega)^{\frac{\varepsilon}{\sigma}}}{\varepsilon} \right) s_{in}(\omega) D_n X_n. \quad (20)$$

Example: Variable Markups in the Quantitative Trade Model

- Combining Equation (10) and (19), we can express $s_{in}(\omega)$ in terms of $c_{in}(\omega)$:

$$\frac{\sigma}{\sigma - s_{in}(\omega)^{\frac{\varepsilon}{\sigma}}} c_{in}(\omega) = \frac{\sigma - 1}{\sigma} \exp\left(\frac{1 - s_{in}(\omega)^{\frac{\varepsilon}{\sigma}}}{\varepsilon}\right) D_n P_n \Rightarrow s_{in}(\omega) = s_n(c_{in}(\omega)) \quad (21)$$

- Then firm ω from country i will serve destination market n if and only if

$$\frac{s_n(c_{in}(\omega))^{\frac{\varepsilon}{\sigma}}}{\sigma} \frac{\sigma - 1}{\sigma} \exp\left(\frac{1 - s_n(c_{in}(\omega))^{\frac{\varepsilon}{\sigma}}}{\varepsilon}\right) s_n(c_{in}(\omega)) D_n X_n \geq w_n F_n \quad (22)$$

- We assume that the cost cut-off c_n^* above which firms from country i will not serve market n satisfies:

$$c_n^* < \min \left\{ \frac{1}{\bar{T}_{in}}, \frac{\sigma - 1}{\sigma} \exp\left(\frac{1}{\varepsilon}\right) D_n P_n \right\}, \quad \forall(i, n) \quad (23)$$

Example: Variable Markups in the Quantitative Trade Model

- Let X_{in} be the total sales of firms originated from country i in destination market n and Π_{in} be the associated profit. Let M_i be the mass of firms in country i

$$\lambda_{in} \equiv \frac{X_{in}}{X_n} = \frac{M_i \bar{T}_{in}^\theta}{\sum_{k=1}^N M_k \bar{T}_{kn}^\theta} \quad (24)$$

$$\frac{\Pi_{in}}{X_{in}} = \eta_n = \frac{\int_0^{c_n^*} \frac{s_n(c)^{\frac{\varepsilon}{\sigma}}}{\sigma} \frac{\sigma-1}{\sigma} \exp\left[\frac{1-s_n(c)^{\frac{\varepsilon}{\sigma}}}{\varepsilon}\right] s_n(c) c^{\theta-1} dc}{\int_0^{c_n^*} \frac{\sigma-1}{\sigma} \exp\left[\frac{1-s_n(c)^{\frac{\varepsilon}{\sigma}}}{\varepsilon}\right] s_n(c) c^{\theta-1} dc} \quad (25)$$

- The price index can be given by

$$P_n = \sum_{i=1}^N \nu_{in}^P M_i \bar{T}_{in}^\theta, \quad \nu_{in}^P \equiv \left[\theta \int_0^{c_n^*} \frac{\sigma}{\sigma - s_n(c)^{\frac{\varepsilon}{\sigma}}} c s_n(c) c^{\theta-1} dc \right] \quad (26)$$

- By the definition of $H(\cdot)$, we have

$$\sum_{i=1}^N M_i \bar{T}_{in}^\theta \theta \int_0^{c_n^*} H(s(c)) c^{\theta-1} dc = 1 \quad (27)$$

Example: Variable Markups in the Quantitative Trade Model

- Equilibrium consists of $(w_i, M_i, P_i, D_i, c_i^*)_{i=1}^N$ such that

1. (w_i) is determined by labor market clearing

$$w_i L_i = \sum_{n=1}^N (1 - \eta_n) \lambda_{in} X_n + w_i F_i (c_i^*)^\theta \sum_{k=1}^N M_k \bar{T}_{ki}^\theta + \sum_{n=1}^N [\eta_n \lambda_{in} X_n - w_n F_n (c_n^*)^\theta M_i \bar{T}_{in}^\theta] \quad (28)$$

2. Firm mass M_i is determined by the free-entry condition:

$$M_i w_i f^e = \sum_{n=1}^N \left[\eta_n \lambda_{in} X_n - w_n F_n (c_n^*)^\theta M_i \bar{T}_{in}^\theta \right] \quad (29)$$

3. Total absorption: $X_i = w_i L_i$
4. The price index is determined by Equation (26)
5. (c_n^*, D_n) are jointly determined by Equation (22) and (27)

Example: Variable Markups in the Quantitative Trade Model

- Draw J numbers from the uniform distribution $U[0, 1]$, sorting them as $u_1 < u_2 < \dots < u_J$
- Initial guess $(w_i, M_i, P_i, D_i)_{i=1}^N$
- Compute the relative quantity cutoff below which firms will not serve the market n by solving:

$$\frac{(s_n^*)^{\frac{\varepsilon}{\sigma}}}{\sigma} \frac{\sigma - 1}{\sigma} \exp\left(\frac{1 - (s_n^*)^{\frac{\varepsilon}{\sigma}}}{\varepsilon}\right) s_n^* D_n X_n = w_n F_n \quad (30)$$

- The cost cutoff can then be computed by

$$c_n^* = \frac{\sigma - (s_n^*)^{\frac{\varepsilon}{\sigma}}}{\sigma} \frac{\sigma - 1}{\sigma} \exp\left(\frac{1 - (s_n^*)^{\frac{\varepsilon}{\sigma}}}{\varepsilon}\right) D_n P_n \quad (31)$$

- Compute \bar{T}_{in} by its definition and λ_{in} by Equation (24)

Example: Variable Markups in the Quantitative Trade Model

- Let $c_n^j = u_j c_n^*$. The corresponding relative quantity s_n^j can be solved by Equation (21)

- Compute

$$\eta_n = \frac{\sum_{j=1}^J \frac{(s_n^j)^{\frac{\varepsilon}{\sigma}}}{\sigma} \exp \left[\frac{1 - (s_n^j)^{\frac{\varepsilon}{\sigma}}}{\varepsilon} \right] s_n^j (c_n^j)^{\theta-1}}{\sum_{j=1}^J \exp \left[\frac{1 - (s_n^j)^{\frac{\varepsilon}{\sigma}}}{\varepsilon} \right] s_n^j (c_n^j)^{\theta-1}} \quad (32)$$

- Compute

$$\nu_n^P = \frac{c_n^*}{J} \sum_{j=1}^J \frac{\theta \sigma}{\sigma - (s_n^j)^{\frac{\varepsilon}{\sigma}}} s_n^j (c_n^j)^{\theta} \quad (33)$$

- Update D_n by:

$$D_n = D_n \times \left[\sum_{i=1}^N M_i \bar{T}_{in}^{\theta} \frac{c_n^*}{J} \theta \sum_{j=1}^J H(s_n^j) (c_n^j)^{\theta-1} \right]^{\frac{1}{1+\theta}} \quad (34)$$

Example: Variable Markups in the Quantitative Trade Model

- (w_i, M_i, P_i) are updated, respectively, by Equation (28), (29), and (26). Repeat until convergence. Notice that we update P_n by the following equation:

$$P_n^{(t+1)} = \left[\left(P_n^{(t)} \right)^{-\theta-1} \nu_n^P \sum_{i=1}^N M_i \bar{T}_{in}^\theta \right]^{-\frac{1}{\theta}} \quad (35)$$

Example: Variable Markups in the Quantitative Trade Model

- Welfare: $U_i = \frac{w_i}{P_i}$
- Aggregate markup: as suggested by [Edmond et al. \(2019\)](#), we compute a sales-weighted harmonic average:

$$\begin{aligned}\bar{\mu}_n^D &:= \left[\theta \left(\sum_{i=1}^N M_i \bar{T}_{in}^\theta \right) \int_0^{c_n^*} \left(\frac{\sigma}{\sigma - s_n(c) \frac{\varepsilon}{\sigma}} \right)^{-1} \frac{p_n(c)}{P_n} s_n(c) c^{\theta-1} dc \right]^{-1} \\ &= \left[\theta \left(\sum_{i=1}^N M_i \bar{T}_{in}^\theta \right) \frac{1}{P_n} \int_0^{c_n^*} s_n(c) c^\theta dc \right]^{-1} \\ &= \left[\frac{\theta}{\nu_n^P} \int_0^{c_n^*} s_n(c) c^\theta dc \right]^{-1}\end{aligned}\tag{36}$$

Example: Variable Markups in the Quantitative Trade Model

- Quantification:
 - How do changes in trade costs, τ_{in} , affect markups in exporting country i as well as importing country n ?
 - How do welfare gains from trade rely on the markup variations? e.g. Comparing with the constant-markup models?

Summary

- Numerical differentiation:
 - Crucial for nonlinear solvers and nonlinear optimization
 - Trade-off between accuracy and efficiency of computation
 - Promising direction: automatic differentiation and deep learning
- Numerical integration:
 - Heterogeneous-agent models
 - Random variables \Rightarrow Moments