Math for Political Scientists Workshop

Day Five: Calculus with Several Variables

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Review Time

- Calculus
- Differential Calculus
- Derivative
- How to get derivative?

Calculus with Several Variables

Motivation

Calculus may allow us to deal with continuous change in a consistent manner, but once there is more than one variable, the question arises of *what* change.

Take, for example, the function $f(x, y, z) = 3xy - y^2z + 2$. When we talk of change in f, to what are we referring?

Partial Derivative

A partial derivative is a derivative where we hold all but one variable constant in a multivariable function. It measures how the function changes as one specific variable changes, while keeping the other variables fixed.

If $f(x_1, x_2, \ldots, x_n)$ is a function of several variables, the partial derivative of f with respect to x_i is denoted by:

$$\frac{\partial f}{\partial x_i}, \quad f'_{x_i}$$

These two notations both indicate that we are differentiating f with respect to x_i, treating all other variables as constants.

Partial Derivative: Formal Definition

Given a function $f(x_1, x_2, \ldots, x_n)$, the partial derivative with respect to x_i is defined as:

$$\frac{\partial f}{\partial x_i} = \lim_{h \to 0} \frac{f(x_1, x_2, \ldots, x_i + h, \ldots, x_n) - f(x_1, x_2, \ldots, x_i, \ldots, x_n)}{h}$$

Example: Partial Derivative with Respect to One Variable

Consider the function $f(x, y) = x^2y + 3xy^2$. To find the partial derivative of f with respect to x, we treat y as a constant:

$$\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}(x^2y + 3xy^2)$$

Differentiating with respect to x:

$$\frac{\partial f}{\partial x} = 2xy + 3y^2$$

Now, find the partial derivative of f with respect to y, treating x as a constant:

$$\frac{\partial f}{\partial y} = \frac{\partial}{\partial y}(x^2y + 3xy^2)$$

Differentiating with respect to y:

$$\frac{\partial f}{\partial y} = x^2 + 6xy$$

Practice

Consider a function $f(x, y, z) = x^2y + yz + z^2x$, find each of the partial derivative of f with respect to x, y, and z.

Practice Solution

1. **Partial Derivative with Respect to x:**

$$\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}(x^2y + yz + z^2x)$$

$$\frac{\partial f}{\partial x} = 2xy + z^2$$

2. **Partial Derivative with Respect to y:**

$$\frac{\partial f}{\partial y} = \frac{\partial}{\partial y}(x^2y + yz + z^2x)$$

$$\frac{\partial f}{\partial y} = x^2 + z$$

Practice Solution

3. **Partial Derivative with Respect to z:**

$$\frac{\partial f}{\partial z} = \frac{\partial}{\partial z}(x^2 y + yz + z^2 x)$$

$$\frac{\partial f}{\partial z} = y + 2zx$$

Gradient Vector

The **gradient vector** is a vector that contains all the partial derivatives of a scalar-valued function.

- It points in the direction of the greatest rate of increase of the function and its magnitude represents the rate of increase in that direction.
- The gradient is a fundamental concept in multivariable calculus and is extensively used in optimization and machine learning.

Gradient Vector: Formal Definition

If $f(x_1, x_2, \ldots, x_n)$ is a scalar-valued function of n variables, the gradient of f is denoted by ∇f and is defined as:

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n} \right)^\top$$

This is a column vector that consists of all the partial derivatives of f with respect to its variables $x_1, x_2, \ldots, x_n$.

Example: Gradient of a Function with Two Variables

Consider the function $f(x, y) = x^2 + 3xy + y^2$. To find the gradient of f, we calculate the partial derivatives with respect to x and y:

1. **Partial Derivative with Respect to x:**

$$\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}(x^2 + 3xy + y^2) = 2x + 3y$$

2. **Partial Derivative with Respect to y:**

$$\frac{\partial f}{\partial y} = \frac{\partial}{\partial y}(x^2 + 3xy + y^2) = 3x + 2y$$

So, the gradient vector ∇f is:

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)^\top = (2x + 3y, 3x + 2y)^\top$$

Total Derivative

The total derivative of a function describes how the function changes with respect to changes in all of its variables.

Suppose you have a function $z = f(x_1, x_2, \ldots, x_n)$, where $x_1, x_2, \ldots, x_n$ are independent variables. The total derivative of z with respect to one of the variables, say t, where each x_i depends on t, can be found using the chain rule.

The total derivative of z with respect to t is given by:

$$\frac{dz}{dt} = \frac{\partial z}{\partial x_1}\frac{dx_1}{dt} + \frac{\partial z}{\partial x_2}\frac{dx_2}{dt} + \cdots + \frac{\partial z}{\partial x_n}\frac{dx_n}{dt} = \sum_{i=1}^{n} \frac{\partial z}{\partial x_i}\frac{dx_i}{dt}$$

Example

Suppose we have a function $z = f(x, y)$, where z depends on the variables x and y, and both x and y depend on another variable t. The total derivative of z with respect to t is given by:

$$\frac{dz}{dt} = \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt}$$

Let's take the following specific function:

$$z = x^3 + 2xy + y^3$$

where $x = t^2 + 1$ and $y = 2t + 3$.

Example Solution (cont.)

1. Step 1: Compute the partial derivatives of z with respect to x and y:

$$\frac{\partial z}{\partial x} = 3x^2 + 2y$$
$$\frac{\partial z}{\partial y} = 2x + 3y^2$$

2. Step 2: Compute the derivatives of x and y with respect to t:

$$\frac{dx}{dt} = 2t$$
$$\frac{dy}{dt} = 2$$

Example Solution

3. Step 3: Substitute these into the formula for the total derivative:

$$\frac{dz}{dt} = \left(3x^2 + 2y\right)\frac{dx}{dt} + \left(2x + 3y^2\right)\frac{dy}{dt}$$

Now, substitute the expressions for x, y, $\frac{dx}{dt}$, and $\frac{dy}{dt}$:

$$\frac{dz}{dt} = \left(3(t^2+1)^2 + 2(2t+3)\right)\cdot 2t + \left(2(t^2+1) + 3(2t+3)^2\right)\cdot 2$$

Simplify the expression:

$$\frac{dz}{dt} = \left(3(t^4 + 2t^2 + 1) + 4t + 6\right)\cdot 2t + \left(2t^2 + 2 + 12t^2 + 36t + 27\right)\cdot 2$$

Expand and combine the terms:

$$\frac{dz}{dt} = 6t^5 + 12t^3 + 36t^2 + 90t + 58$$

Practice:

Suppose we have a function $z = f(x, y)$, where z depends on the variables x and y, and both x and y depend on another variable t. The total derivative of z with respect to t is given by:

$$\frac{dz}{dt} = \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt}$$

Let's take the following specific function:

$$z = x^2 + 3xy + y^2$$

where $x = t^2$ and $y = t + 1$.

Practice Solution (cont.):

1. Step 1: Compute the partial derivatives of z with respect to x and y:

$$\frac{\partial z}{\partial x} = 2x + 3y$$
$$\frac{\partial z}{\partial y} = 3x + 2y$$

2. Step 2: Compute the derivatives of x and y with respect to t:

$$\frac{dx}{dt} = 2t$$
$$\frac{dy}{dt} = 1$$

Practice Solution:

3. Step 3: Substitute these into the formula for the total derivative:

$$\frac{dz}{dt} = (2x + 3y)\frac{dx}{dt} + (3x + 2y)\frac{dy}{dt}$$

Now, substitute the expressions for x, y, $\frac{dx}{dt}$, and $\frac{dy}{dt}$:

$$\frac{dz}{dt} = \left(2t^2 + 3(t+1)\right) \cdot 2t + \left(3t^2 + 2(t+1)\right) \cdot 1$$

Simplify the expression:

$$\frac{dz}{dt} = \left(2t^2 + 3t + 3\right) \cdot 2t + \left(3t^2 + 2t + 2\right)$$

Expand and combine the terms:

$$\frac{dz}{dt} = 4t^3 + 9t^2 + 8t + 2$$

Jacobian Matrix

Simple Description

- The Jacobian matrix is a matrix that represents all the first-order partial derivatives of a vector-valued function.
- If you have a function that takes several inputs and gives several outputs, the Jacobian matrix captures how small changes in each input affect each output.

Jacobian Matrix (cont.)

Formal Presentation

Suppose you have a vector-valued function $\mathbf{F} : \mathbb{R}^n \to \mathbb{R}^m$ defined as:

$$\mathbf{F}(\mathbf{x}) = \begin{pmatrix} f_1(x_1, x_2, \ldots, x_n) \\ f_2(x_1, x_2, \ldots, x_n) \\ \vdots \\ f_m(x_1, x_2, \ldots, x_n) \end{pmatrix}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top$ is a vector of inputs.

Jacobian Matrix

The Jacobian matrix $\mathbf{J}(\mathbf{x})$ of the function $\mathbf{F}$ is an $m \times n$ matrix where each element J_{ij} is the partial derivative of the i-th function with respect to the j-th variable:

$$\mathbf{J}(\mathbf{x}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{pmatrix}$$

Example: Simple 2x2 Case

Consider a function $\mathbf{F} : \mathbb{R}^2 \to \mathbb{R}^2$ defined as:

$$\mathbf{F}(x, y) = \begin{pmatrix} f_1(x, y) \\ f_2(x, y) \end{pmatrix} = \begin{pmatrix} x^2 + y \\ xy \end{pmatrix}$$

The Jacobian matrix $\mathbf{J}$ of this function is calculated by taking the partial derivatives of each function with respect to x and y:

$$\mathbf{J}(x, y) = \begin{pmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{pmatrix} = \begin{pmatrix} 2x & 1 \\ y & x \end{pmatrix}$$

So, for this example, the Jacobian matrix is:

$$\mathbf{J}(x, y) = \begin{pmatrix} 2x & 1 \\ y & x \end{pmatrix}$$

Hessian Matrix

The **Hessian matrix** is a square matrix that organizes all the possible second-order partial derivatives of a function with multiple variables.

- This matrix helps us understand the curvature of the function in different directions.
- In simpler terms, the Hessian matrix tells us how the function bends or curves around a particular point in space.

Hessian Matrix: Formal Definition

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a function that maps an n-dimensional vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ to a real number.

The Hessian matrix $H(f)$ of the function f is an $n \times n$ matrix, where the element in the i-th row and j-th column is the second-order partial derivative of f with respect to x_i and x_j.

Mathematically, the Hessian matrix $H(f)$ is defined as:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Example: Hessian Matrix

Consider the function $f(x, y) = x^2 + y^2$.

First, we find the first-order partial derivatives:

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial f}{\partial y} = 2y$$

Next, we find the second-order partial derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial y^2} = 2, \quad \frac{\partial^2 f}{\partial x \partial y} = 0$$

(and similarly, $\frac{\partial^2 f}{\partial y \partial x} = 0$).

So, the Hessian matrix for this function is:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

Example: Hessian Matrix

Consider the function $f(x, y, z) = xy + yz + zx$.

First, we find the first-order partial derivatives:

$$\frac{\partial f}{\partial x} = y + z, \quad \frac{\partial f}{\partial y} = x + z, \quad \frac{\partial f}{\partial z} = x + y$$

Next, we find the second-order partial derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 0, \quad \frac{\partial^2 f}{\partial y^2} = 0, \quad \frac{\partial^2 f}{\partial z^2} = 0$$

$$\frac{\partial^2 f}{\partial x \partial y} = 1, \quad \frac{\partial^2 f}{\partial x \partial z} = 1, \quad \frac{\partial^2 f}{\partial y \partial z} = 1$$

(and similarly, $\frac{\partial^2 f}{\partial y \partial x} = 1$, $\frac{\partial^2 f}{\partial z \partial x} = 1$, $\frac{\partial^2 f}{\partial z \partial y} = 1$).

So, the Hessian matrix for this function is:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial z \partial x} & \frac{\partial^2 f}{\partial z \partial y} & \frac{\partial^2 f}{\partial z^2} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

A Slightly Complex Linear Practice

Consider the function $f(x, y, z) = 2x^2 + 3xy + 4yz + 5zx$, find the Hessian matrix of $f(x, y, z)$.

Practice Solution (cont.)

1. Step 1: First-Order Partial Derivatives

First, we compute the first-order partial derivatives:

$$\frac{\partial f}{\partial x} = 4x + 3y + 5z$$
$$\frac{\partial f}{\partial y} = 3x + 4z$$
$$\frac{\partial f}{\partial z} = 4y + 5x$$

Practice Solution (cont.)

2. Step 2: Second-Order Partial Derivatives

Next, we compute the second-order partial derivatives:

- For x:

$$\frac{\partial^2 f}{\partial x^2} = 4$$
$$\frac{\partial^2 f}{\partial x \partial y} = 3$$
$$\frac{\partial^2 f}{\partial x \partial z} = 5$$

- For y:

$$\frac{\partial^2 f}{\partial y^2} = 0$$
$$\frac{\partial^2 f}{\partial y \partial z} = 4$$

- For z:

$$\frac{\partial^2 f}{\partial z^2} = 0$$

Practice Solution

3. Step 3: Construct the Hessian Matrix

The Hessian matrix is:

$$H(f) = \begin{bmatrix} 4 & 3 & 5 \\ 3 & 0 & 4 \\ 5 & 4 & 0 \end{bmatrix}$$

Wrap-Up Time

- Partial derivative
- Gradient
- Total derivative
- Jacobian matrix
- Hessian Matrix

Applications in Political Methodology

eg.,

- Multivariate Regression (PLSC 503)
- Maximum Likelihood Estimation (PLSC 503 and 504)

Well done, everyone!

You should be proud of yourself!

Good luck with your first semester!