

Taylor Expansion

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1 Taylor Expansion

Any real infinitely differentiable function $f(x)$ at a given point a can be expressed in terms of its Taylor series:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} (x-a)^n = f(a) + f'(a)(x-a) + \frac{1}{2}f''(a)(x-a)^2 + \frac{1}{6}f'''(a)(x-a)^3 + \dots$$

or equivalently the function $f(x+h)$ at the point x :

$$f(x+h) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x)}{n!} h^n = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(x)h^3 + \dots$$

This allows us to approximate $f(x)$ with a polynomial up to a chosen order. For example, $f(x)$ can be approximated at $x=a$ as the polynomial of order 2, i.e. the quadratic:

$$f(x+h) \approx f(x) + f'(x)h + \frac{1}{2}f''(x)h^2$$

In many applications, including data assimilation, we often require the linear approximation:

$$f(x+h) \approx f(x) + f'(x)h$$

1.1 Multivariable Taylor Expansion

To extend the above concept of a linear approximation to functions of two variables in order to approximate $f(x+a, y+b)$ at the point (x, y) , we require partial derivatives:

$$f(x+\delta x, y+\delta y) \approx f(x, y) + f_x(x, y)\delta x + f_y(x, y)\delta y$$

where $f_x(x, y)$ and $f_y(x, y)$ are the partial derivatives of $f(x, y)$ with respect to x and y respectively. It follows that a vector of functions:

$$\mathbf{f}(\mathbf{x}) = \begin{pmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{pmatrix}$$

can be approximated at a point $\mathbf{x} = (x, y)$ in a similar way:

$$\mathbf{f}(\mathbf{x} + \delta \mathbf{x}) = \begin{pmatrix} f_1(x+\delta x, y+\delta y) \\ f_2(x+\delta x, y+\delta y) \end{pmatrix} \approx \begin{pmatrix} f_1(x, y) + \frac{\partial f_1}{\partial x}(x, y)\delta x + \frac{\partial f_1}{\partial y}(x, y)\delta y \\ f_2(x, y) + \frac{\partial f_2}{\partial x}(x, y)\delta x + \frac{\partial f_2}{\partial y}(x, y)\delta y \end{pmatrix} = \mathbf{f}(\mathbf{x}) + \mathbb{J}(\mathbf{f}, \mathbf{x})\delta \mathbf{x}$$

where $\delta \mathbf{x} = \begin{pmatrix} \delta x \\ \delta y \end{pmatrix}$ and $\mathbb{J}(\mathbf{f}, \mathbf{x})$ is the Jacobian:

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

The linear approximation

$$\mathbf{f}(\mathbf{x} + \delta \mathbf{x}) \approx \mathbf{f}(\mathbf{x}) + \mathbb{J}(\mathbf{f}, \mathbf{x})\delta \mathbf{x}$$

also applies for higher dimensions where

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

Higher order Taylor expansions, for the quadratic approximation for instance, would require calculation of the Hessian in addition to the Jacobian.

1.2 Taylor Expansion for Compound Functions

Consider the compound function $\mathbf{f} \circ \mathbf{g}(\mathbf{x}) = \mathbf{f}(\mathbf{g}(\mathbf{x}))$ for $\mathbf{f} : \mathbb{R}^n \mapsto \mathbb{R}^m$ and $\mathbf{g} : \mathbb{R}^n \mapsto \mathbb{R}^n$. The Taylor expansion is given by

$$\mathbf{f}(\mathbf{g}(\mathbf{x} + \delta \mathbf{x})) = \mathbf{f}(\mathbf{g}(\mathbf{x})) + \mathbb{J}(\mathbf{f} \circ \mathbf{g}, \mathbf{x})\delta \mathbf{x} = \mathbf{f}(\mathbf{g}(\mathbf{x})) + \mathbb{J}(\mathbf{f}, \mathbf{g})\mathbb{J}(\mathbf{g}, \mathbf{x})\delta \mathbf{x}$$

where we have used

$$\begin{aligned} \mathbb{J}(\mathbf{f} \circ \mathbf{g}, \mathbf{x}) &= \begin{pmatrix} \frac{\partial(\mathbf{f} \circ \mathbf{g})_1}{\partial x_1} & \frac{\partial(\mathbf{f} \circ \mathbf{g})_1}{\partial x_2} & \cdots & \frac{\partial(\mathbf{f} \circ \mathbf{g})_1}{\partial x_n} \\ \frac{\partial(\mathbf{f} \circ \mathbf{g})_2}{\partial x_1} & \frac{\partial(\mathbf{f} \circ \mathbf{g})_2}{\partial x_2} & \cdots & \frac{\partial(\mathbf{f} \circ \mathbf{g})_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial(\mathbf{f} \circ \mathbf{g})_m}{\partial x_1} & \frac{\partial(\mathbf{f} \circ \mathbf{g})_m}{\partial x_2} & \cdots & \frac{\partial(\mathbf{f} \circ \mathbf{g})_m}{\partial x_n} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial f_1}{\partial g_1} \frac{\partial g_1}{\partial x_1} + \cdots + \frac{\partial f_1}{\partial g_n} \frac{\partial g_n}{\partial x_1} & \frac{\partial f_1}{\partial g_1} \frac{\partial g_1}{\partial x_2} + \cdots + \frac{\partial f_1}{\partial g_n} \frac{\partial g_n}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial g_1} \frac{\partial g_1}{\partial x_n} + \cdots + \frac{\partial f_1}{\partial g_n} \frac{\partial g_n}{\partial x_n} \\ \frac{\partial f_2}{\partial g_1} \frac{\partial g_1}{\partial x_1} + \cdots + \frac{\partial f_2}{\partial g_n} \frac{\partial g_n}{\partial x_1} & \frac{\partial f_2}{\partial g_1} \frac{\partial g_1}{\partial x_2} + \cdots + \frac{\partial f_2}{\partial g_n} \frac{\partial g_n}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial g_1} \frac{\partial g_1}{\partial x_n} + \cdots + \frac{\partial f_2}{\partial g_n} \frac{\partial g_n}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial g_1} \frac{\partial g_1}{\partial x_1} + \cdots + \frac{\partial f_m}{\partial g_n} \frac{\partial g_n}{\partial x_1} & \frac{\partial f_m}{\partial g_1} \frac{\partial g_1}{\partial x_2} + \cdots + \frac{\partial f_m}{\partial g_n} \frac{\partial g_n}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial g_1} \frac{\partial g_1}{\partial x_n} + \cdots + \frac{\partial f_m}{\partial g_n} \frac{\partial g_n}{\partial x_n} \end{pmatrix} \\ &= \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} \begin{pmatrix} \frac{\partial g_1}{\partial x_1} & \frac{\partial g_1}{\partial x_2} & \cdots & \frac{\partial g_1}{\partial x_n} \\ \frac{\partial g_2}{\partial x_1} & \frac{\partial g_2}{\partial x_2} & \cdots & \frac{\partial g_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g_m}{\partial x_1} & \frac{\partial g_m}{\partial x_2} & \cdots & \frac{\partial g_m}{\partial x_n} \end{pmatrix} \\ &= \mathbb{J}(\mathbf{f}, \mathbf{g})\mathbb{J}(\mathbf{g}, \mathbf{x}) \end{aligned} \tag{1}$$

It follows that for any number of compounded functions

$$\mathbf{f} \circ \mathbf{g}_1 \circ \cdots \circ \mathbf{g}_p(\mathbf{x} + \delta \mathbf{x}) = \mathbf{f} \circ \mathbf{g}_1 \circ \cdots \circ \mathbf{g}_p(\mathbf{x}) + \mathbb{J}(\mathbf{f}, \mathbf{g}_1)\mathbb{J}(\mathbf{g}_1, \mathbf{g}_2)\cdots\mathbb{J}(\mathbf{g}_p, \mathbf{x})\delta \mathbf{x}$$

where $\mathbf{f} : \mathbb{R}^n \mapsto \mathbb{R}^m$ and $\mathbf{g}_i : \mathbb{R}^n \mapsto \mathbb{R}^n$ for $i = 1, \dots, p$.