

# Memo

## Hyperdual numbers

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### 1 Hyperdual numbers

This memo briefly describes the implementation of hyperdual numbers for the purpose of differentiation. The concept of hyperdual numbers is described by Rehner and Bauer [2] and Fike and Alonso [1].

Third order hyperdual number,

$$x = x_0 + x_1\epsilon_1 + x_2\epsilon_2 + x_3\epsilon_3 + x_{12}\epsilon_{12} + x_{13}\epsilon_{13} + x_{23}\epsilon_{23} + x_{123}\epsilon_{123} \quad (1)$$

The exact Taylor expansion of  $f(x, y, z)$  using hyperdual numbers,

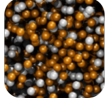
$$\begin{aligned} f(x + \epsilon_1, y + \epsilon_2, z + \epsilon_3) = & f^0 + f_x^0\epsilon_1 + f_y^0\epsilon_2 + f_z^0\epsilon_3 \\ & + f_{xy}^0\epsilon_1\epsilon_2 + f_{xz}^0\epsilon_1\epsilon_3 + f_{yz}^0\epsilon_2\epsilon_3 \\ & + f_{xyz}^0\epsilon_1\epsilon_2\epsilon_3 \end{aligned} \quad (2)$$

Taylor expansion of function  $f(x)$  yields

$$\begin{aligned} f(x) = & f(x_0) + f'(x_0)x_1\epsilon_1 + f'(x_0)x_2\epsilon_2 + f'(x_0)x_3\epsilon_3 \\ & + f'(x_0)x_{12}\epsilon_{12} + f'(x_0)x_{13}\epsilon_{13} + f'(x_0)x_{23}\epsilon_{23} \\ & + f'(x_0)x_{123}\epsilon_{123} \\ & + f''(x_0)x_1x_2\epsilon_1\epsilon_2 + f''(x_0)x_1x_3\epsilon_1\epsilon_3 + f''(x_0)x_2x_3\epsilon_2\epsilon_3 \\ & + f''(x_0)x_1x_{23}\epsilon_1\epsilon_{23} + f''(x_0)x_{12}x_3\epsilon_{12}\epsilon_3 + f''(x_0)x_2x_{13}\epsilon_2\epsilon_{13} \\ & + f'''(x_0)x_1x_2x_3\epsilon_1\epsilon_2\epsilon_3. \end{aligned} \quad (3)$$

Note that the prefactors  $1/2$  and  $1/3$  cancels. Gathering terms,

$$\begin{aligned} f(x) = & f(x_0) + f'(x_0)x_1\epsilon_1 + f'(x_0)x_2\epsilon_2 + f'(x_0)x_3\epsilon_3 \\ & + \left( f'(x_0)x_{12} + f''(x_0)x_1x_2 \right) \epsilon_1\epsilon_2 \\ & + \left( f'(x_0)x_{13} + f''(x_0)x_1x_3 \right) \epsilon_1\epsilon_3 \\ & + \left( f'(x_0)x_{23} + f''(x_0)x_2x_3 \right) \epsilon_2\epsilon_3 \\ & + \left( f'(x_0)x_{123} + f''(x_0)(x_1x_{23} + x_{12}x_3 + x_2x_{13}) + f'''(x_0)x_1x_2x_3 \right) \epsilon_1\epsilon_2\epsilon_3. \end{aligned} \quad (4)$$



Multiplication of two numbers,

$$\begin{aligned}
 xy = & x_0y_0 + (x_0y_1 + x_1y_0) \epsilon_1 + (x_0y_2 + x_2y_0) \epsilon_2 + (x_0y_3 + x_3y_0) \epsilon_3 \\
 & + (x_0y_{12} + x_{12}y_0 + x_1y_2 + x_2y_1) \epsilon_1\epsilon_2 \\
 & + (x_0y_{13} + x_{13}y_0 + x_1y_3 + x_3y_1) \epsilon_1\epsilon_3 \\
 & + (x_0y_{23} + x_{23}y_0 + x_2y_3 + x_3y_2) \epsilon_2\epsilon_3 \\
 & + (x_0y_{123} + x_{123}y_0 + x_{12}y_3 + x_3y_{12} + x_{13}y_2 + x_{23}y_1 + x_{23}y_1) \epsilon_1\epsilon_2\epsilon_3.
 \end{aligned} \tag{5}$$

## 1.1 Needed differentials

Differentials to third order is required for the most common functions.

### 1.1.1 Exponential function ( $\exp(x)$ )

$$f(x) = \exp(x) = f'(x) = f''(x) = f'''(x) \tag{6}$$

### 1.1.2 Sine function ( $\sin(x)$ )

$$f(x) = \sin(x) \tag{7}$$

$$f'(x) = \cos(x) \tag{8}$$

$$f''(x) = -\sin(x) \tag{9}$$

$$f'''(x) = -\cos(x) \tag{10}$$

### 1.1.3 Cosine function ( $\cos(x)$ )

$$f(x) = \cos(x) \tag{11}$$

$$f'(x) = -\sin(x) \tag{12}$$

$$f''(x) = -\cos(x) \tag{13}$$

$$f'''(x) = \sin(x) \tag{14}$$

### 1.1.4 Tangent function ( $\tan(x)$ )

$$f(x) = \tan(x) \tag{15}$$

$$f'(x) = \sec^2(x) = \tan^2(x) + 1 \tag{16}$$

$$f''(x) = 2 \tan(x) \sec^2(x) \tag{17}$$

$$f'''(x) = 2 \sec^2(x)(\sec^2(x) + 2 \tan^2(x)) \tag{18}$$

### 1.1.5 Natural logarithm ( $\log(x)$ )

$$f(x) = \log(x) \tag{19}$$

$$f'(x) = \frac{1}{x} \tag{20}$$

$$f''(x) = -\frac{1}{x^2} \tag{21}$$

$$f'''(x) = \frac{2}{x^3} \tag{22}$$



### 1.1.6 Inverse cosine function ( $\text{acos}(x)$ )

$$f(x) = \text{acos}(x) \quad (23)$$

$$f'(x) = -\frac{1}{\sqrt{1-x^2}} \quad (24)$$

$$f''(x) = -\frac{x}{(1-x^2)^{3/2}} \quad (25)$$

$$f'''(x) = \frac{-2x^2-1}{(1-x^2)^{5/2}} \quad (26)$$

### 1.1.7 Inverse sine function ( $\text{asin}(x)$ )

$$f(x) = \text{asin}(x) \quad (27)$$

$$f'(x) = \frac{1}{\sqrt{1-x^2}} \quad (28)$$

$$f''(x) = \frac{x}{(1-x^2)^{3/2}} \quad (29)$$

$$f'''(x) = \frac{2x^2+1}{(1-x^2)^{5/2}} \quad (30)$$

### 1.1.8 Inverse tangent function ( $\text{atan}(x)$ )

$$f(x) = \text{atan}(x) \quad (31)$$

$$f'(x) = \frac{1}{1+x^2} \quad (32)$$

$$f''(x) = \frac{-2x}{(x^2+1)^2} \quad (33)$$

$$f'''(x) = \frac{6x^2-2}{(x^2+1)^3} \quad (34)$$

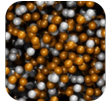
### 1.1.9 Power function ( $x^a$ )

$$f(x) = x^a \quad (35)$$

$$f'(x) = ax^{a-1} \quad (36)$$

$$f''(x) = a(a-1)x^{a-2} \quad (37)$$

$$f'''(x) = a(a-1)(a-2)x^{a-3} \quad (38)$$



## References

- [1] Jeffrey Fike and Juan Alonso. The Development of Hyper-Dual Numbers for Exact Second-Derivative Calculations. In *49th AIAA Aerosp. Sci. Meet. New Horiz. Forum Aerosp. Expo.*, Orlando, Florida, January 2011. American Institute of Aeronautics and Astronautics. ISBN 978-1-60086-950-1. doi: 10.2514/6.2011-886.
- [2] Philipp Rehner and Gernot Bauer. Application of Generalized (Hyper-) Dual Numbers in Equation of State Modeling. *Front. Chem. Eng.*, 3:758090, 2021. doi: 10.3389/fceng.2021.758090.