Thermotools memo

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https://thermotools.github.io/thermopack/index.html

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,

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

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

$$\begin{aligned} f\left(x+\epsilon_1, y+\epsilon_2, z+\epsilon_3\right) = {} & f^0 + f^0_x\epsilon_1 + f^0_y\epsilon_2 + f^0_z\epsilon_3 \\ & + f^0_{xy}\epsilon_1\epsilon_2 + f^0_{xz}\epsilon_1\epsilon_3 + f^0_{yz}\epsilon_2\epsilon_3 \\ & + f^0_{xyz}\epsilon_1\epsilon_2\epsilon_3 \end{aligned} \tag{2}$$

Taylor expansion of function $f(x)$ yields

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

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

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

Multiplication of two numbers,

$$\begin{aligned}
xy = {} & x_0y_0 + (x_0y_1 + x_1y_0)\,\epsilon_1 + (x_0y_2 + x_2y_0)\,\epsilon_2 + (x_0y_3 + x_3y_0)\,\epsilon_3 \\
& + (x_0y_{12} + x_{12}y_0 + x_1y_2 + x_2y_1)\,\epsilon_1\epsilon_2 \\
& + (x_0y_{13} + x_{13}y_0 + x_1y_3 + x_3y_1)\,\epsilon_1\epsilon_3 \\
& + (x_0y_{23} + x_{23}y_0 + x_3y_2 + x_2y_3)\,\epsilon_2\epsilon_3 \\
& + (x_0y_{123} + x_{123}y_0 + x_{12}y_3 + x_3y_{12} + x_{13}y_2 + x_2y_{13} + x_{23}y_1 + x_{23}y_1)\,\epsilon_1\epsilon_2\epsilon_3. \qquad (5)
\end{aligned}$$

1.1 Needed differenitials

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

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

$$f(x) = \exp(x) = f'(x) = f''(x) = f'''(x) \qquad (6)$$

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

$$f(x) = \sin(x) \qquad (7)$$
$$f'(x) = \cos(x) \qquad (8)$$
$$f''(x) = -\sin(x) \qquad (9)$$
$$f'''(x) = -\cos(x) \qquad (10)$$

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

$$f(x) = \cos(x) \qquad (11)$$
$$f'(x) = -\sin(x) \qquad (12)$$
$$f''(x) = -\cos(x) \qquad (13)$$
$$f'''(x) = \sin(x) \qquad (14)$$

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

$$f(x) = \tan(x) \qquad (15)$$
$$f'(x) = \sec^2(x) = \tan^2(x) + 1 \qquad (16)$$
$$f''(x) = 2\tan(x)\sec^2(x) \qquad (17)$$
$$f'''(x) = 2\sec^2(x)(\sec^2(x) + 2\tan^2(x)) \qquad (18)$$

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

$$f(x) = \log(x) \qquad (19)$$
$$f'(x) = \frac{1}{x} \qquad (20)$$
$$f''(x) = -\frac{1}{x^2} \qquad (21)$$
$$f'''(x) = \frac{2}{x^3} \qquad (22)$$

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

$$f(x) = \mathrm{acos}(x) \tag{23}$$
$$f'(x) = -\frac{1}{\sqrt{1+x^2}} \tag{24}$$
$$f''(x) = -\frac{x}{(1-x^2)^{3/2}} \tag{25}$$
$$f'''(x) = \frac{-2x^2-1}{(1-x^2)^{5/2}} \tag{26}$$

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

$$f(x) = \mathrm{asin}(x) \tag{27}$$
$$f'(x) = \frac{1}{\sqrt{1+x^2}} \tag{28}$$
$$f''(x) = \frac{x}{(1-x^2)^{3/2}} \tag{29}$$
$$f'''(x) = \frac{2x^2+1}{(1-x^2)^{5/2}} \tag{30}$$

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

$$f(x) = \mathrm{atan}(x) \tag{31}$$
$$f'(x) = \frac{1}{1+x^2} \tag{32}$$
$$f''(x) = \frac{-2x}{(x^2+1)^2} \tag{33}$$
$$f'''(x) = \frac{6x^2-2}{(x^2+1)^3} \tag{34}$$

1.1.9 Power function (x^a)

$$f(x) = x^a \tag{35}$$
$$f'(x) = ax^{a-1} \tag{36}$$
$$f''(x) = a(a-1)x^{a-2} \tag{37}$$
$$f'''(x) = a(a-1)(a-2)x^{a-3} \tag{38}$$

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.