# Chain rule

Just like the composition in C++ classes, we have composition of functions.

| | | | |
|---|---|---|---|
| $(f \circ g)(x)$ | $\equiv$ | $f(g(x))$ | univariate |
| $(f \circ g)(x,y)$ | $\equiv$ | $f(g(x,y))$ | bivariate |
| $(f \circ g)(x,y,z)$ | $\equiv$ | $f(g(x,y,z))$ | trivariate |

Then we have **univariate** chain rule for first derivative :

$$(f \circ g)'(x) = f'(g)g'(x)$$

And also the **univariate** chain rules for higher order derivatives : (terms are groups by $f''(g)$, $f'''(g)$, $f''''(g)$)

$$(f \circ g)''(x) = f''(g)(g'(x))^2 + f'(g)g''(x)$$
$$(f \circ g)'''(x) = f'''(g)(g'(x))^3 + f'(g)g'''(x) + 3f''(g)g''(x)g'(x)$$
$$(f \circ g)''''(x) = f''''(g)(g'(x))^4 + f'(g)g''''(x) + 6f'''(g)g''(x)(g'(x))^2 + f''(g)[4g'''(x)g'(x) + 3(g''(x))^2]$$

**Flawed** proof of 1st derivative

$$\begin{aligned}
(f \circ g)'(x) &= \lim_{y\to x} \frac{(f \circ g)(y) - (f \circ g)(x)}{y - x} \\
&= \lim_{y\to x} \frac{(f \circ g)(y) - (f \circ g)(x)}{g(y) - g(x)} \frac{g(y) - g(x)}{y - x} \\
&= \lim_{y\to x} \frac{(f \circ g)(y) - (f \circ g)(x)}{g(y) - g(x)} \lim_{y\to x} \frac{g(y) - g(x)}{y - x} && \text{flaw : violates algebraic limit theorem} \\
&= f'(g)g'(x) && \text{flaw : } f'(g) \equiv \lim_{\Delta\to 0} \frac{f(g(x)+\Delta) - f(g(x))}{\Delta} \neq \lim_{\Delta\to 0} \frac{f(g(x+\Delta)) - f(g(x))}{\Delta}
\end{aligned}$$

Recall the algebraic limit theorem

| | | | |
|---|---|---|---|
| $\lim_{x\to c}(f(x)+g(x))$ | = | $\lim_{x\to c} f(x) + \lim_{x\to c} g(x)$ | if $\lvert\lim_{x\to c} f(x)\rvert < \infty$ or $\lvert\lim_{x\to c} g(x)\rvert < \infty$ |
| $\lim_{x\to c}(f(x)-g(x))$ | = | $\lim_{x\to c} f(x) - \lim_{x\to c} g(x)$ | if $\lvert\lim_{x\to c} f(x)\rvert < \infty$ or $\lvert\lim_{x\to c} g(x)\rvert < \infty$ |
| $\lim_{x\to c}(f(x)\times g(x))$ | = | $\lim_{x\to c} f(x) \times \lim_{x\to c} g(x)$ | if $\lvert\lim_{x\to c} f(x)\rvert < \infty$ or $\lvert\lim_{x\to c} g(x)\rvert < \infty$ |
| $\lim_{x\to c}(f(x)\div g(x))$ | = | $\lim_{x\to c} f(x) \div \lim_{x\to c} g(x)$ | if ($\lvert\lim_{x\to c} f(x)\rvert < \infty$ or $\lvert\lim_{x\to c} g(x)\rvert < \infty$) and $\lim_{x\to c} g(x) \neq 0$ |

Proof of 1st derivative

- define $u = (g(x+\Delta x) - g(x))/\Delta x - g'(x)$ (1)
- define $v = (f(y+\Delta y) - f(y))/\Delta y - f'(y)$ (2)
- since $g'(x) = \lim_{\Delta x\to 0}(g(x+\Delta x) - g(x))/\Delta x$ hence $\lim_{\Delta x\to 0} u = 0$
- since $f'(y) = \lim_{\Delta y\to 0}(f(y+\Delta y) - f(y))/\Delta y$ hence $\lim_{\Delta y\to 0} v = 0$

from (1) $g(x+\Delta x) = g(x) + (g'(x)+u)\Delta x$ (3)
from (2) $f(y+\Delta y) = f(y) + (f'(y)+v)\Delta y$ (4)

$$\begin{aligned}
& \lim_{\Delta x\to 0}[f(g(x+\Delta x)) - f(g(x))]/\Delta x \\
=\ & \lim_{\Delta x\to 0}[f(g(x) + (g'(x)+u)\Delta x) - f(g(x))]/\Delta x && \text{from (4)} \\
=\ & \lim_{\Delta x\to 0}[f(g(x)) + (f'(g(x))+v)(g'(x)+u)\Delta x - f(g(x))]/\Delta x && \text{from (3) with } \Delta y = (g'(x)+u)\Delta x \\
=\ & \lim_{\Delta x\to 0}(f'(g(x))+v)(g'(x)+u) \\
=\ & \lim_{\Delta x\to 0}(f'(g(x))+v)\lim_{\Delta x\to 0}(g'(x)+u) \\
=\ & (\lim_{\Delta x\to 0} f'(g(x)) + \lim_{\Delta x\to 0} v)(\lim_{\Delta x\to 0} g'(x) + \lim_{\Delta x\to 0} u) \\
=\ & f'(g(x))g'(x)
\end{aligned}$$

Proof of 2nd derivative

$$
\begin{aligned}
(f\circ g)''(x) &= \frac{d(f\circ g)'(x)}{dx} \\
&= \frac{d(f'(g)g'(x))}{dx} && \text{(from 1st derivative)} \\
&= f''(g)g'(x)g'(x)+f'(g)g''(x) \\
&= f''(g)(g'(x))^2+f'(g)g''(x)
\end{aligned}
$$

Proof of 3rd derivative

$$
\begin{aligned}
(f\circ g)'''(x) &= \frac{d(f\circ g)''(x)}{dx} \\
&= \frac{d(f''(g)(g'(x))^2+f'(g)g''(x))}{dx} && \text{(from 2nd derivative)} \\
&= f'''(g)g'(x)(g'(x))^2+2f''(g)g'(x)g''(x)+f''(g)g'(x)g''(x)+f'(g)g'''(x) \\
&= f'''(g)(g'(x))^3+f'(g)g'''(x)+3f''(g)g''(x)g'(x)
\end{aligned}
$$

Proof of 4th derivative

$$
\begin{aligned}
(f\circ g)''''(x) &= \frac{d(f\circ g)'''(x)}{dx} \\
&= \frac{d(f'''(g)(g'(x))^3+f'(g)g'''(x)+3f''(g)g''(x)g'(x))}{dx} && \text{(from 3rd derivative)} \\
&= f''''(g)g'(x)(g'(x))^3+3f'''(g)(g'(x))^2g''(x)+f''(g)g'(x)g'''(x)+f'(g)g''''(x)+ \\
&\quad 3f'''(g)g'(x)g''(x)g'(x)+3f''(g)[g'''(x)g'(x)+g''(x)g''(x)] \\
&= f''''(g)(g'(x))^4+3f'''(g)g''(x)(g'(x))^2+f''(g)g'''(x)g'(x)+f'(g)g''''(x)+ \\
&\quad 3f'''(g)g''(x)(g'(x))^2+3f''(g)g'''(x)g'(x)+3f''(g)(g''(x))^2 \\
&= f''''(g)(g'(x))^4+f'(g)g''''(x)+6f'''(g)g''(x)(g'(x))^2+f''(g)[4g'''(x)g'(x)+3(g''(x))^2]
\end{aligned}
$$

**Derivative of inverse function**

With chain rule, we can derive the 1st derivative of inverse function.

$$
\begin{aligned}
x &= (f^{-1}\circ f)(x) \\
dx/dx &= (f^{-1}\circ f)'(x) \\
1 &= f^{-1}{}'(f)f'(x) && \text{by chain rule for 1st derivative} \\
f^{-1}{}'(f) &= 1/f'(x)
\end{aligned}
$$

With chain rule, we can derive the 2nd derivative of inverse function.

$$
\begin{aligned}
x &= (f^{-1}\circ f)(x) \\
d^2x/dx^2 &= (f^{-1}\circ f)''(x) \\
0 &= f^{-1}{}''(f)(f'(x))^2+f^{-1}{}'(f)f''(x) && \text{by chain rule for 2nd derivative} \\
f^{-1}{}''(f) &= -f^{-1}{}'(f)f''(x)(f'(x))^{-2} \\
&= -f''(x)(f'(x))^{-3} && \text{since } f^{-1}{}'(f) = 1/f'(x)
\end{aligned}
$$

With chain rule, we can derive the 3rd derivative of inverse function.

$$
\begin{aligned}
x &= (f^{-1}\circ f)(x) \\
d^3x/dx^3 &= (f^{-1}\circ f)'''(x) \\
0 &= f^{-1}{}'''(f)(f'(x))^3+f^{-1}{}'(f)f'''(x)+3f^{-1}{}''(f)f''(x)f'(x) && \text{by chain rule for 3rd derivative} \\
f^{-1}{}'''(f) &= -f^{-1}{}'(f)f'''(x)(f'(x))^{-3}-3f^{-1}{}''(f)f''(x)f'(x)(f'(x))^{-3} \\
&= -f'''(x)(f'(x))^{-4}-3f^{-1}{}''(f)f''(x)(f'(x))^{-4} && \text{since } f^{-1}{}'(f) = 1/f'(x) \\
&= -f'''(x)(f'(x))^{-4}+3(f''(x))^2(f'(x))^{-5} && \text{since } f^{-1}{}''(f) = -f''(x)(f'(x))^{-3}
\end{aligned}
$$

Summary

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

$$f^{-1}{}''(f) = -\frac{f''(x)}{f'(x)^3}$$

$$f^{-1}{}'''(f) = -\frac{f'''(x)}{f'(x)^4} + 3\frac{f''(x)^2}{f'(x)^5}$$

Example

$$y = f(x) = x^n$$

$$x = f^{-1}(y) = y^{1/n}$$

Method 1 : using ordinary differentiation

$$f'(x) = nx^{n-1}$$

$$f''(x) = n(n-1)x^{n-2}$$

$$f'''(x) = n(n-1)(n-2)x^{n-3}$$

$$f^{-1}{}'(y) = \frac{1}{n}y^{\frac{1-n}{n}}$$

$$f^{-1}{}''(y) = \frac{1}{n}\frac{1-n}{n}y^{\frac{1-2n}{n}}$$

$$f^{-1}{}'''(y) = \frac{1}{n}\frac{1-n}{n}\frac{1-2n}{n}y^{\frac{1-3n}{n}}$$

Method 2 : using inverse function’s derivative formula

$$f^{-1}{}'(y) = \frac{1}{f'(x)} = \frac{1}{nx^{n-1}}$$

$$= \frac{1}{n}x^{1-n} \qquad \text{in terms of } x$$

$$= \frac{1}{n}y^{\frac{1-n}{n}} \qquad \text{in terms of } y$$

$$f^{-1}{}''(y) = -\frac{f''(x)}{f'(x)^3} = -\frac{n(n-1)x^{n-2}}{n^3x^{3n-3}}$$

$$= \frac{1-n}{n^2}x^{1-2n} \qquad \text{in terms of } x$$

$$= \frac{1}{n}\frac{1-n}{n}y^{\frac{1-2n}{n}} \qquad \text{in terms of } y$$

$$f^{-1}{}'''(y) = -\frac{f'''(x)}{f'(x)^4} + 3\frac{f''(x)^2}{f'(x)^5} = -\frac{n(n-1)(n-2)x^{n-3}}{n^4x^{4n-4}} + 3\frac{n^2(n-1)^2x^{2n-4}}{n^5x^{5n-5}}$$

$$= -\frac{(n-1)(n-2)}{n^3}x^{1-3n} + 3\frac{(n-1)^2}{n^3}x^{1-3n}$$

$$= \frac{3(n-1)^2 - (n-1)(n-2)}{n^3}x^{1-3n}$$

$$= \frac{(n-1)((3n-3)-(n-2))}{n^3}x^{1-3n}$$

$$= \frac{(n-1)(2n-1)}{n^3}x^{1-3n} \qquad \text{in terms of } x$$

$$= \frac{1}{n}\frac{1-n}{n}\frac{1-2n}{n}y^{\frac{1-3n}{n}} \qquad \text{in terms of } y$$

Both methods give the same set of results.