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A CHAIN RULE FOR DIFFERENTIATION WITH APPLICATIONS TO MULTIVARIATE HERMITE POLYNOMIALS

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A chain rule is given for differentiating a multivariate function of a multivariate function. In the univariate case this chain rule reduces to Faa de Bruno's formula.

Using this, a simple procedure is given to obtain the rth order multivariate Hermite polynomial from the rth order univariate Hermite polynomial.

1. The chain rule

The following formula for the derivatives of a function of a function is easily verified.

For $f : R^c \to R^d$, $g : R^d \to R^e$, $\pi = (\alpha_1, \ldots, \alpha_r)$ a set of r integers in $\{1, 2, \ldots, c\}$ and x in R^c , set $y = f(x)$, and $(f)_\pi(x) = \partial^r f(x)/\partial x_{\alpha_1} \ldots \partial x_{\alpha_r}$; then $(g \circ f)(x) = g(f(x))$ has rth order derivatives

$$(g \circ f)_\pi(x) = \sum_{k=1}^{r} (g)_{i_1 \ldots i_k}(y) \sum_\pi (f_{i_1})_{\pi_1}(x) \ldots (f_{i_k})_{\pi_k}(x) ,$$

where summation as each $i_1, \ldots, i_k$ ranges over 1 to d is implicit,

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and $\sum_{\pi}$ sums over all partitions $(\pi_1, \ldots, \pi_k)$ of π.

If the number of sets $\pi_1, \ldots, \pi_k$ of length i is n_i, $1 \le i \le r$, then $n_1 + 2n_2 + \ldots + rn_r = r$, $n_1 + \ldots + n_r = k$, and the number of such partitions is $m(n) = r! \,/\, \prod_{i=1}^{r} \left(i!^{n_i} n_i! \right)$. Hence we may write $\sum_{\pi} = \sum_{n} \sum^{m(n)}$, where $\sum^{m(n)}$ sums over all $m(n)$ such partitions of π and $\sum_{n}$ sums over all such n.

EXAMPLE. If $r = 4$, the possibilities are

n_1	n_2	n_3	n_4	k	$m(n)$
0	0	0	1	1	1
1	0	1	0	2	4
0	2	0	0	2	3
2	1	0	0	3	6
4	0	0	0	4	1 ;

hence

$$
\begin{aligned}
(g \circ f)_{\alpha_1 \ldots \alpha_4}(x) = {} & (g)_{i_1} (f_{i_1})_{\alpha_1 \ldots \alpha_4} \\
& + (g)_{i_1 i_2} \left\{ \sum^{4} (f_{i_1})_{\alpha_1} (f_{i_2})_{\alpha_2 \alpha_3 \alpha_4} + \sum^{3} (f_{i_1})_{\alpha_1 \alpha_2} (f_{i_2})_{\alpha_3 \alpha_4} \right\} \\
& + (g)_{i_1 i_2 i_3} \sum^{6} (f_{i_1})_{\alpha_1} (f_{i_2})_{\alpha_2} (f_{i_3})_{\alpha_3 \alpha_4} \\
& + (g)_{i_1 i_2 i_3 i_4} (f_{i_1})_{\alpha_1} (f_{i_2})_{\alpha_2} (f_{i_3})_{\alpha_3} (f_{i_4})_{\alpha_4} ,
\end{aligned}
$$

where $(g)_{\pi} = (g)_{\pi}(y)$ and $(f_i)_{\pi} = (f_i)_{\pi}(x)$. □

If $c = d = 1$ this becomes Faa de Bruno's formula

$$(g \circ f)^{(r)}(x) = \sum_{k=1}^{r} g^{(k)}(y) \sum_{n} m(n) f^{(1)}(x)^{n_1} \ldots f^{(r)}(x)^{n_r} ,$$

where $f^{(r)}(x) = (d/dx)^r f(x)$; see Goursat [2, p. 34].

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2. The multivariate Hermite polynomials

The rth univariate Hermite polynomial is defined as

$$He_r(x) = \exp\left(x^2/2\right)(-d/dx)^r \exp\left(-x^2/2\right) \ , \quad r \geq 0 \ . \quad x \text{ in } R \ .$$

The first 10 are given in Kendall and Stuart [3, p. 155]. For example,

$$He_5(x) = x^5 - 10x^3 + 15x \ .$$

Let $A = \left(A_{ij}\right)$ be any symmetric $c \times c$ matrix, x any point in R^c, and $\alpha = \left(\alpha_1, \ldots, \alpha_r\right)$, where for $1 \leq i \leq r$, α_i is any number in $\{1, 2, \ldots, c\}$. Then the general rth order Hermite polynomial is

$$He_\alpha(x, A) = (-)^r \exp(Q/2) \left(\partial^r / \partial x_{\alpha_1} \ldots \partial x_{\alpha_r}\right) \exp(-Q/2) \ , \text{ where } Q = x'Ax \ .$$

These polynomials are the building block for multivariate Edgeworth expansions.

(For some results on these see Erdelyi [1, p. 285]; his notation is different.) An expression for $He_\alpha(x, A)$ follows immediately from that of $He_r(x)$. This is best illustrated by an example. From $He_5(x)$ above it follows that, for $r = 5$,

$$He_\alpha(x, A) = W_{\alpha_1} \ldots W_{\alpha_5} - \sum^{10} W_{\alpha_1} W_{\alpha_2} W_{\alpha_3} A_{\alpha_4\alpha_5} + \sum^{15} W_{\alpha_1} A_{\alpha_2\alpha_3} A_{\alpha_4\alpha_5} \ ,$$

where

$$W_i = \sum_{j=1}^{r} A_{ij} x_j$$

and

$$\sum^{m} W_{a_1} \ldots W_{a_l} A_{b_1 b_2} \ldots A_{b_{2k-1} b_{2k}} = \sum^{m} I_{l,2k}(a, b)$$

say, denotes the sum over all $m = (l+2k)!/\left(l!2^k k!\right)$ partitions a, b of α of length l and $2k$ respectively, allowing for the symmetry of A. For example

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$$\sum^3 W_a A_{bc} = W_a A_{bc} + W_b A_{ca} + W_c A_{ab} \ .$$

The general formula

$$He_\alpha(x, A) = \sum_{l+2k=r} (-)^k \sum^m I_{l,2k}(a, b)$$

follows from §1.

References

[1] A. Erdelyi, *Higher transcendental functions*, volume 2 (McGraw-Hill, New York, 1953).

[2] E. Goursat, *A course in mathematical analysis*, volume 1 (Dover, New York, 1959).

[3] M.G. Kendall and A. Stuart, *The advanced theory of statistics*, volume 1, second edition (Griffin, London, 1963).

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