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nth-order derivatives of certain inverses and the Bell polynomials

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Abstract. By employing certain concepts in combinatorial analysis, we derive here the closed-form expressions for the nth-order derivatives of the following:
(i) inverse powers of a matrix $\mathscr{A}$
(ii) reciprocal powers of a function f (explicit or implicit)
(iii) reciprocal powers of a determinant A
and establish their relation with the Bell polynomials.

1. Introduction

It is generally believed that Leibnitz's theorem for the product of two functions (say, $f \cdot g$) holds true for the quotient as well (say, f/g), as regards the closed form for its nth-order derivative. However, this is not true and we shall show in this paper in detail that the nth-order derivative of inverse† powers of the following:

(i) a matrix $\mathscr{A}$
(ii) a function f (explicit or implicit)
(iii) a determinant A

do enjoy closed-form expressions of their own.

To accomplish this task, we require the following basic concepts which arise in a study of the various 'arrangements' possible for an integral number n (Riordan 1958).

(i) Partition. By definition, this is a collection of integers (with a given sum) without regard to order.

(ii) Composition. The 'ordered' collection of integers (with a given sum) is called composition.

In our earlier paper (Singh 1987), we have used the results derived in section 3 of the present paper to arrive at a closed-form expression for the infinite sum occurring in the evaluation of the single-clipped correlation.

2. nth-order derivative of a matrix inverse $D^n\mathscr{A}^{-1}$

The starting point is the identity

$$\mathscr{A}\mathscr{A}^{-1} = [I] \tag{1}$$

where the elements of $\mathscr{A}$ and $\mathscr{A}^{-1}$ are functions of a single parameter, say x.

† Used in the general sense that we have, $\theta^r\theta^{-r} = \text{identity}$, where θ stands for $\mathscr{A}$, f or A and $r \geqslant 1$.

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Applying Leibnitz's theorem to this product, we get

$$\mathrm{D}^n(\mathscr{A}\mathscr{A}^{-1}) = \sum_{j=0}^{n} {}^nC_j \mathrm{D}^j\mathscr{A}\mathrm{D}^{n-j}\mathscr{A}^{-1} = \mathrm{D}^n[I] = [0] \tag{2}$$

where $\mathrm{D}^n = \mathrm{d}^n/\mathrm{d}x^n$.

From (2) it follows that†

$$-\mathrm{D}^n(\mathscr{A}^{-1}) = {}^nC_1\mathscr{A}^{-1}\mathrm{D}^1\mathscr{A}\mathrm{D}^{n-l}\mathscr{A}^{-1} + {}^nC_2\mathscr{A}^{-1}\mathrm{D}^2\mathscr{A}\mathrm{D}^{n-2}\mathscr{A}^{-1} + \ldots$$
$$+ {}^nC_k\mathscr{A}^{-1}\mathrm{D}^k\mathscr{A}\mathrm{D}^{n-k}\mathscr{A}^{-1} + \ldots + {}^nC_n\mathscr{A}^{-1}\mathrm{D}^n\mathscr{A}\mathscr{A}^{-1}. \tag{3}$$

Introducing the notation $\mathscr{P}_k = \mathscr{A}^{-1}\mathrm{D}^k\mathscr{A}$, we can arrive at the following expressions for particular values of n (say, $n = 1, 2, 3, 4$):

$n = 1$

$$\mathrm{D}^1\mathscr{A}^{-1} = -\mathscr{P}_1^1\mathscr{A}^{-1} = \left((-1)^1\frac{\mathscr{P}_1}{1!}\right)\mathscr{A}^{-1}$$

$n = 2$

$$\mathrm{D}^2\mathscr{A}^{-1} = (2\mathscr{P}_1^2 - \mathscr{P}_2)\mathscr{A}^{-1} = 2!\left[(-1)^2\left(\frac{\mathscr{P}_1}{1!}\right)^2 + (-1)^1\frac{\mathscr{P}_2}{2!}\right]\mathscr{A}^{-1}$$

$n = 3$

$$\mathrm{D}^3\mathscr{A}^{-1} = [-6\mathscr{P}_1^3 + 3(\mathscr{P}_1\mathscr{P}_2 + \mathscr{P}_2\mathscr{P}_1) - \mathscr{P}_3]\mathscr{A}^{-1}$$
$$= 3!\left[(-1)^3\left(\frac{\mathscr{P}_1}{1!}\right)^3 + (-1)^2\left(\frac{\mathscr{P}_1}{1!}\frac{\mathscr{P}_2}{2!} + \frac{\mathscr{P}_2}{2!}\frac{\mathscr{P}_1}{1!}\right) + (-1)^1\frac{\mathscr{P}_3}{3!}\right]\mathscr{A}^{-1}$$

$n = 4$

$$\mathrm{D}^4\mathscr{A}^{-1} = [24\mathscr{P}_1^4 - 12(\mathscr{P}_1^2\mathscr{P}_2 + \mathscr{P}_1\mathscr{P}_2\mathscr{P}_1 + \mathscr{P}_2\mathscr{P}_1^2) + 6\mathscr{P}_2^2 + 4(\mathscr{P}_1\mathscr{P}_3 + \mathscr{P}_3\mathscr{P}_1) - \mathscr{P}_4]\mathscr{A}^{-1}$$
$$= 4!\left\{(-1)^4\left(\frac{\mathscr{P}_1}{1!}\right)^4 + (-1)^3\left[\left(\frac{\mathscr{P}_1}{1!}\right)^2\left(\frac{\mathscr{P}_2}{2!}\right) + \frac{\mathscr{P}_1}{1!}\frac{\mathscr{P}_2}{2!}\frac{\mathscr{P}_1}{1!} + \frac{\mathscr{P}_2}{2!}\left(\frac{\mathscr{P}_1}{1!}\right)^2\right]\right.$$
$$\left. + (-1)^2\left[\left(\frac{\mathscr{P}_2}{2!}\right)^2 + \frac{\mathscr{P}_1}{1!}\frac{\mathscr{P}_3}{3!} + \frac{\mathscr{P}_3}{3!}\frac{\mathscr{P}_1}{1!}\right] + (-1)^1\frac{\mathscr{P}_4}{4!}\right\}\mathscr{A}^{-1}. \tag{4}$$

From the equations above, it can be seen clearly that the general result is

$$\mathrm{D}^n\mathscr{A}^{-1} = n!\left(\sum_{k=1}^{n}(-1)^k\frac{\mathscr{P}_{i_l}}{i_l!}\frac{\mathscr{P}_{i_2}}{i_2!}\cdots\frac{\mathscr{P}_{i_k}}{i_k!}\right)\mathscr{A}^{-1} \tag{5}$$

where $\mathscr{P}_i = \mathscr{A}^{-1}\mathrm{D}^i\mathscr{A}$ and the summation is taken over all the integers $(i_1, i_2, \ldots, i_k > 0)$ distinct or otherwise, such that $\Sigma_{m=1}^{k} i_m = n$.

† Bodewig (1958, p 36), expands $\mathrm{D}^n(\mathscr{A}^{-1})$ with the fundamental mistake of assuming that all $\mathrm{D}^n\mathscr{A} = 0$ for $n > 1$.

Proceeding exactly in the same manner, we can easily generalise the result of (5) to

$$\mathrm{D}^n\mathscr{A}^{-r} = n!\left(\sum_{k=1}^{n} (-1)^k \frac{\mathscr{P}_{i_1}}{i_1!}\frac{\mathscr{P}_{i_2}}{i_2!}\cdots\frac{\mathscr{P}_{i_k}}{i_k!}\right)\mathscr{A}^{-r} \tag{6}$$

where now, $\mathscr{P}_i = \mathscr{A}^{-r}\mathrm{D}^i\mathscr{A}^r$ $(r \geq 1)$ and the summation is done as in (5).

The number of permutations of the various i_m in (6) above depends on how many times a 'distinct' i_m $(i_1 \neq i_2 \neq \ldots \neq i_k)$ occurs in the sum $\Sigma_{m=1}^{k} i_m = n$. Let l_m determine the frequency with which a distinct i_m occurs, then the number of permutations for each partition of n with a fixed k is given by

$$\nu(k; l_1, l_2, \ldots, l_k) = \frac{k!}{l_1!\, l_2! \ldots l_k!}$$
$$\sum_m l_m = k \qquad \sum_m l_m i_m = n. \tag{7}$$

For example, when $n = 7$ and $k = 3$, we have the following four partitions:

I	II	III	IV
3, 3, 1	3, 2, 2	4, 2, 1	5, 1, 1

Thus we find that whereas there are only two distinct numbers i_m with $m = 1, 2$ constituting partitions I, II and IV, partition III consists of three distinct numbers i_m with $m = 1, 2, 3$. The numbers of permutations in these four partitions are

$$\nu_{\mathrm{I}}(3; 2, 1) = \nu_{\mathrm{II}}(3; 1, 2) = \nu_{\mathrm{IV}}(3; 1, 2) = \frac{3!}{2!1!} = \frac{3!}{1!2!} = 3$$
$$\nu_{\mathrm{III}}(3; 1, 1, 1) = \frac{3!}{1!1!1!} = 6. \tag{8}$$

Further, on summing over all the permutations above, we should get the total number of compositions of the number $n = 7$ with $k = 3$,

$$\nu_{\mathrm{I}}(3; 2, 1) + \nu_{\mathrm{II}}(3; 1, 2) + \nu_{\mathrm{III}}(3; 1, 1, 1) + \nu_{\mathrm{IV}}(3; 1, 2)$$
$$= 3 + 3 + 6 + 3 = 15$$
$$= \frac{6!}{4!2!} = \binom{7-1}{3-1}. \tag{9}$$

In general (see Riordan 1968):

$$\sum_{\Sigma_m l_m = k, \Sigma_m l_m i_m = n} \nu(k; l_1, l_2, \ldots, l_k) = \sum_{\Sigma_m l_m = k, \Sigma_m l_m i_m = n} \frac{k!}{l_1!\, l_2! \ldots l_k!} = \binom{n-1}{k-1}. \tag{10}$$

Finally, the total number of compositions of n for all the k is given by (Riordan 1968):

$$\sum_{k=1}^{n} \binom{n-1}{k-1} = 2^{n-1}. \tag{11}$$

2.1. *The generating function (GF) for $\mathrm{D}^n\mathscr{A}^{-r}$*

From (6), it is apparent that the required nature of the GF should be such that it generates all the compositions of n, or equivalently, should generate all the partitions of n occurring in various permutations for each k where $1 \leqslant k \leqslant n$. We see that the 'ordinary' Bell polynomials $\hat{B}_{n,k}$ (Comtet 1974, p 136) satisfy the above specifications:

$$\sum_{i \geqslant 1} (x_i t^i)^k = \sum_{n \geqslant k} \hat{B}_{n,k}(x_1, x_2, \ldots, x_k) t^n \tag{12}$$

where $x_i = \mathscr{P}_i / i!$. From (12), the following relation becomes apparent:

$$\hat{B}_{n,k}(x_1, x_2, \ldots, x_k) = \sum (x_{i_1})(x_{i_2}) \ldots (x_{i_k}) \tag{13}$$

and the summation over all the integers $(i_1, i_2, \ldots, i_k > 0)$ distinct or otherwise, is done in the same manner as in (5). Therefore, the closed form for $\mathrm{D}^n \mathscr{A}^{-r}$ $(r \geqslant 1)$ as obtained from (6) and (13) now takes the following compact form:

$$\mathrm{D}^n \mathscr{A}^{-r} = n! \left(\sum_{k=1}^{n} (-1)^k \hat{B}_{n,k} \right) \mathscr{A}^{-r}$$

where

$$\hat{B}_{n,k} = \hat{B}_{n,k}\left(\frac{\mathscr{P}_1}{1!}, \frac{\mathscr{P}_2}{2!}, \ldots, \frac{\mathscr{P}_k}{k!} \right) \qquad \mathscr{P}_k = \mathscr{A}^{-r} \mathrm{D}^k \mathscr{A}^r. \tag{14}$$

2.2. Generation of $D^{n+1}\mathscr{A}^{-r}$ from $D^n \mathscr{A}^{-r}$ $(r \geqslant 1)$

We first observe that given $\mathscr{P}_k = \mathscr{A}^{-r} \mathrm{D}^k \mathscr{A}^r$, we have

$$\mathrm{D}\mathscr{P}_k = -\mathscr{P}_1 \mathscr{P}_k + \mathscr{P}_{k+1}. \tag{15}$$

Differentiation of (14) coupled with (15) implies that $n![\Sigma_{k=1}^{n} (-1)^k (\mathrm{D}\hat{B}_{n,k} - \hat{B}_{n,k}\mathscr{P}_1)]\mathscr{A}^{-r}$ should result in $(n+1)![\Sigma_{k=1}^{n+1} (-1)^k \hat{B}_{n+1,k}]\mathscr{A}^{-r}$ after complete evaluation. But unfortunately, there is no simple recurrence relation between $\mathrm{D}\hat{B}_{n,k}$ and $\hat{B}_{n+1,k}$ so that the above expressions could be shown to be the same in an independent manner as well. We shall, however, show this for a particular value of n (say, $n = 3$) explicitly. First,

$$\begin{aligned} 3! \sum_{k=1}^{3} (-1)^k \mathrm{D}\hat{B}_{3,k} & \\ &= 3![(-1)^3 \mathrm{D}\hat{B}_{3,3} + (-1)^2 \mathrm{D}\hat{B}_{3,2} + (-1)^1 \mathrm{D}\hat{B}_{3,1}] \\ &= [(-1)^4 18\mathscr{P}_1^4 + (-1)^3 (12\mathscr{P}_1^2\mathscr{P}_2 + 9\mathscr{P}_1\mathscr{P}_2\mathscr{P}_1 + 9\mathscr{P}_2\mathscr{P}_1^2) \\ &\quad + (-1)^2 (6\mathscr{P}_2^2 + 4\mathscr{P}_1\mathscr{P}_3 + 4\mathscr{P}_3\mathscr{P}_1) + (-1)^1 \mathscr{P}_4] \end{aligned} \tag{16}$$

and

$$3! \sum_{k=1}^{3} (-1)^{k+1} \hat{B}_{3,k}\mathscr{P}_1 = [(-1)^4 6\mathscr{P}_1^4 + (-1)^3 3(\mathscr{P}_1\mathscr{P}_2\mathscr{P}_1 + \mathscr{P}_2\mathscr{P}_1^2) + (-1)^2 \mathscr{P}_3\mathscr{P}_1]. \tag{17}$$

Addition of (16) and (17) gives us

$$\begin{aligned} 3! \sum_{k=1}^{3} (\mathrm{D}\hat{B}_{3,k} - \hat{B}_{3,k}\mathscr{P}_1) & \\ &= 4! \left\{ (-1)^4 \left(\frac{\mathscr{P}_1}{1!} \right)^4 + (-1)^3 \left[\left(\frac{\mathscr{P}_1}{1!} \right)^2 \frac{\mathscr{P}_2}{2!} + \frac{\mathscr{P}_1}{1!} \frac{\mathscr{P}_2}{2!} \frac{\mathscr{P}_1}{1!} + \frac{\mathscr{P}_2}{2!} \left(\frac{\mathscr{P}_1}{1!} \right)^2 \right] \right. \\ &\quad \left. + (-1)^2 \left[\left(\frac{\mathscr{P}_2}{2!} \right)^2 + \frac{\mathscr{P}_1}{1!} \frac{\mathscr{P}_3}{3!} + \frac{\mathscr{P}_3}{3!} \frac{\mathscr{P}_1}{1!} \right] + (-1)^1 \frac{\mathscr{P}_4}{4!} \right\} \\ &= 4![(-1)^4 \hat{B}_{4,4} + (-1)^3 \hat{B}_{4,3} + (-1)^2 \hat{B}_{4,2} + (-1)^1 \hat{B}_{4,1}] \end{aligned}$$

$$= 4!\left(\sum_{k=1}^{4} (-1)^4 \hat{B}_{4,k}\right)$$

which generates $D^{n+1}\mathscr{A}^{-r}$ from $D^n\mathscr{A}^{-r}$ when $n = 3$.

3. *n*th-order derivative of the inverse of a function $D^n f^{-1}$

In the equation for $D^n\mathscr{A}^{-1}$, if the matrix $\mathscr{A}$ is replaced by an ordinary function f, we see that all the permutations (see (7)) coalesce into just one number and the ordinary Bell polynomials $\hat{B}_{n,k}$ will now be replaced by the exponential Bell polynomials $B_{n,k}$, which are defined as follows. Consider the expansion of $e^P D^n e^{-P}$ where $e^P = f$. If we note that $DP = f^{-1}Df = Dff^{-1} = P_1$ and that $DP_k = -P_1P_k + P_{k+1}$ where $P_k = f^{-1}D^k f = D^k f f^{-1}$, we find that

$$e^P D^n e^{-P} = B_n = \sum_{k=1}^{n} (-1)^k k!\, B_{n,k}(P_1, P_2, \ldots, P_{n-k+1}). \tag{18}$$

The exponential Bell polynomials $B_{n,k}$ also have the following multinomial form (Comtet 1974, p 134):

$$B_{n,k}(P_1, P_2, \ldots, P_{n-k+1}) = \sum_{\Sigma_{j=1}^{n} i_j = k,\, \Sigma_{j=1}^{n} j i_j = n} \left(\frac{n!}{i_1!\, i_2! \ldots 1^{i_1} 2^{i_2} \ldots}\right) P_1^{i_1} P_2^{i_2} \ldots . \tag{19}$$

But as $e^P D^n e^{-P} = f D^n f^{-1}$, we get from (18) that

$$D^n f^{-1} = \left(\sum_{k=1}^{n} (-1)^k k!\, B_{n,k}\right) f^{-1} \tag{20}$$

where the parentheses in $B_{n,k}$ above are dopped for convenience.

3.1. $D^{n+1} f^{-1}$ *by induction*

On differentiating (18), we find the following recurrence relations:

$$B_{n+1} = DB_n - P_1 B_n \tag{21}$$

$$B_{n+1,k} = DB_{n,k} + P_1 B_{n,k-1} \tag{22}$$

where $P_1 = B_{1,1}$; $B_{n,k} = 0$ if $k = 0$ and $B_{n,n} = (B_{1,1})^n$. Now, from (18) and (22), $D^{n+1} f^{-1}$ follows immediately:

$$D^{n+1} f^{-1} = \sum_{k=1}^{n} (-1)^k k!\,(DB_{n,k} - P_1 B_{n,k}) f^{-1}$$

$$= \sum_{k=1}^{n} (-1)^k k!\,(B_{n+1,k} - P_1 B_{n,k-1} - P_1 B_{n,k}) f^{-1}$$

$$= \sum_{k=1}^{n+1} [(-1)^k k!\, B_{n+1,k}] f^{-1} \tag{23}$$

as can be easily seen on expansion.

Thus in the case of a function, it is possible to show directly that if a form is true for $D^n f^{-1}$, it is true for $D^{n+1} f^{-1}$ as well.

3.2. $D^n(f^{-r})$ when $r>1$

It becomes immediately apparent from the expression for $D^n(\mathscr{A}^{-r})$ that now for $D^n(f^{-r})$, the multiplying factor in the summand on the right-hand side will be ${}^{k+r-1}C_k$. Thus, we get the following expression for $D^n(f^{-r})$:

$$D^n(f^{-r}) = \left(\sum_{k=1}^{n} (-1)^k \frac{(k+r-1)!}{(r-1)!} B_{n,k}\right) f^{-r} \tag{24}$$

where for $r=1$ we regain (20).

Such formulae as given above have been discussed by Comtet (1974, theorem B, p 141) where the final expression for $D^n(f^{-r})$ is given in terms of the Laurent series rather than the compact form given in (24).

4. *n*th-order derivative of the inverse of a composite function

The case of the nth-order derivative of a composite function is known—the famous Faa' di Bruno's formula (see Riordan 1958, pp 34–8). However, our task here is to show what the nth-order derivative of the 'inverse' case would look like.

Let $f(u)$ be the composite function such that

$$u = g(x) \qquad f_i = f^{-1}(u) D_u^i f(u) \qquad g_i = g^{-1}(x) D_x^i g(x). \tag{25}$$

Then, following Gibson (1958), the expression for the nth-order derivative of the inverse of a composite function can be expressed as

$$D_x^n[f^{-1}(n)] = \sum_{k=1}^{n} \frac{A_{n,k}(x)}{k!} D_u^k[f^{-1}(u)] \tag{26}$$

where

$$A_{n,k}(x) = \sum_{i=0}^{k-1} (-1)^i \, {}^kC_i u^i D_x^n u^{k-i}. \tag{27}$$

Now, if we utilise the form for $D_u^k[f^{-1}(u)]$ as given by (20), we get the closed-form expression for $D_x^n[f^{-1}(u)]$. The other way is to identify $A_{n,k}/k!$ with the exponential Bell polynomials as done in Riordan (1958, pp 35–8) and we find that

$$\frac{A_{n,k}}{k!} = B_{n,k}. \tag{28}$$

Thus from (20), (25), (26) and (28), it follows that

$$D_x^n[f^{-1}(u)] = \left[\sum_{k=1}^{n} B_{n,k}^x \left(\sum_{p=1}^{k} (-1)^p p! B_{k,p}^u\right)\right] f^{-1}(u) \tag{29}$$

where the superscripts x and u in $B_{n,k}$ and $B_{k,p}$, respectively, specify the differentiations.

The required GF for (29) is

$$\frac{1}{k!}\left[\sum_{i\geq 1}\left(\frac{g_i t^i}{i!}\right)\right]^k \left[\sum_{j\geq 1}(-1)^j\left(\frac{f_j t^j}{j!}\right)\right]^p$$

as the coefficients of $(t^n/n!)(t^k/k!)$ in the above sum are the summands on the right-hand side of (29).

5. *n*th-order derivative of the inverse of a determinant $D^n A^{-r}$

The results of section 3 are also valid for the nth-order derivative of the inverse of a determinant A if we replace f by A in (20) and (24). But on realising the cumbersome nature of determinant algebra, it is preferable to use the following identity due to Bodewig (1958, p 41):

$$DA = A\,\mathrm{Tr}(\mathscr{A}^{-1}D\mathscr{A}). \tag{30}$$

Applying Leibnitz's theorem twice to the right-hand side of (30) and using (14), we get

$$\begin{aligned} D^k A &= \sum_{j=0}^{k-1} \sum_{p=0}^{k-1-j} \frac{(k-1)!}{j!\,p!\,(k-1-j-p)!} D^j A\,\mathrm{Tr}[D^p(\mathscr{A}^{-1})D^{k-j-p}(\mathscr{A})] \\ &= \sum_{j=0}^{k-1} \sum_{p=0}^{k-1-j} \frac{(k-1)!}{j!\,(k-1-j-p)!} D^j A\,\mathrm{Tr}\left[\left(\sum_{q=1}^{p} (-1)^q \hat{B}_{p,q}\right)\mathscr{P}_{k-j-p}\right]. \end{aligned} \tag{31}$$

In (31), we notice that whenever $p=0$, we just have $\mathscr{A}^{-1}$ instead of the complete expansion for $D^p(\mathscr{A}^{-1})$.

Now, to obtain the final expression for $D^n(A^{-r})$, we simply put $A=f$ in (24) where $P_i = A^{-1}D^iA = D^iAA^{-1}$ and D^kA is given by (31).

7. Conclusion

Thus we see that the closed-form expressions derived above are valid for any arbitrary power of the following:

(i) inverse of a matrix
(ii) inverse of an ordinary function
(iii) inverse of a composite function
(iv) inverse of a determinant

and are expressible in terms of the Bell polynomials (ordinary or exponential).

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