Problem 3. Let g be a smooth function, i.e. a function which has derivatives of all orders. Recall that $g^{(k)}$ denotes the k-th derivative of g. For non-negative integers n, k, define the function $T_{n,k}(x)$ as follows:

$$T_{n,k}(x) = \sum_{j=0}^{n} \binom{n}{j} (-1)^{n-j} g^{n-j}(x)(g^j)^{(k)}(x)$$

(we set $g^0 = 1$). For example, $T_{3,3}(x) = 3g^2(x)g^{(3)}(x) - 3g(x)(g^2)^{(3)}(x) + (g^3)^{(3)}(x)$.

a) Prove that $T_{n,k}(x) = 0$ for any $n > k$ and any x.

b) Find a simple explicit formula for $T_{n,n}(x)$ (for example, $T_{3,3}(x) = 6(g'(x))^3$. Check this!).

Solution. We start with the beautiful solution submitted by Prof. Valdislav Kargin.

First solution (after Slava Kargin). The binomial theorem tells us that

$$(g(y) - g(x))^n = \sum_{j=0}^{n} \binom{n}{j} (-1)^{n-j} g^{n-j}(x) g^j(y).$$

Taking k-th derivative with respect to y we get:

$$\frac{d^k}{dy^k}(g(y) - g(x))^n = \sum_{j=0}^{n} \binom{n}{j} (-1)^{n-j} g^{n-j}(x)(g^j)^{(k)}(y).$$

It follows that

$$T_{n,k}(x) = \frac{d^k}{dy^k}(g(y) - g(x))^n|_{y=x} = (h^n)^{(k)}(x),$$

where $h(y) = g(y) - g(x)$ (we think of y as a variable and x as fixed here). Note that $h(x) = 0$ and $h'(y) = g'(y)$. Let us compute the first few derivatives of $h^n(y)$ to see a pattern:

$$(h^n)'(y) = nh^{n-1}(y)h'(y) = h^{n-1}(y)b_1(y),$$

where $b_1(y) = nh'(y) = ng'(y)$. Then

$$(h^n)''(y) = (n-1)h^{n-2}(y)h'(y)b_1(y) + h^{n-1}(y)b_1'(y) = h^{n-2}(y)b_2(y),$$

where $b_2(y) = (n-1)g'(y)b_1(y) + h(y)b_1'(y)$. Next

$$(h^n)^{(3)}(y) = (n-2)h^{n-3}(y)h'(y)b_2(y) + h^{n-2}(y)b_2'(y) = h^{n-3}(y)b_3(y),$$

where $b_3(y) = (n-2)g'(y)b_2(y) + h(y)b_2'(y)$.

Now it is easy to see the pattern: for $k \le n$, the k-th derivative of $h^n(y)$ is of the form $h^{n-k}(y)b_k(y)$ for some smooth function b_k. It is a simple exercise to prove this by induction on k. This immediately implies that $T_{n,k}(x) = (h^n)^{(k)}(x) = h^{n-k}(x)b_k(x) = 0$ for $k < n$ (since $h(x) = 0$). This proves the first part of the problem. To answer the second part, note that $T_{n,n}(x) = b_n(x)$ and that

$$b_k(y) = (n-k+1)g'(y)b_{k-1}(y) + h(y)b_{k-1}'(y)$$

for $1 < k \le n$. It follows that $b_k(x) = (n-k+1)g'(x)b_{k-1}(x)$ for $1 < k \le n$ (since $h(x) = 0$). A simple induction yields $b_k(x) = n(n-1)\dots(n-k+1)(g'(x))^k$ for $1 \le k \le n$. Thus

$$T_{n,n}(x) = b_n(x) = n!(g'(x))^n.$$

Second solution. In problems of this type one often tries to find first some relations between the functions $T_{n,k}$ when n, k vary in hope to get some recursive formulas an apply induction.

Let us try to see what the derivative of $T_{n,k}$ is:

$$T_{n,k}'(x) = \sum_{j=0}^{n} \binom{n}{j} (-1)^{n-j} [g^{n-j}(x)(g^j)^{(k)}(x)]'.$$

Using the product rule, we see that

$$[g^{n-j}(x)(g^j)^{(k)}(x)]' = [g^{n-j}(x)]'(g^j)^{(k)}(x) + g^{n-j}(x)(g^j)^{(k+1)}(x) =$$

$$(n-j)g^{n-j-1}(x)g'(x)(g^j)^{(k)}(x) + g^{n-j}(x)(g^j)^{(k+1)}(x).$$

It follows that

$$T'_{n,k}(x) = \sum_{j=0}^{n} \binom{n}{j}(-1)^{n-j}(n-j)g^{n-j-1}(x)g'(x)(g^j)^{(k)}(x) + \sum_{j=0}^{n} \binom{n}{j}(-1)^{n-j}g^{n-j}(x)(g^j)^{(k+1)}(x) =$$

$$-g'(x)\sum_{j=0}^{n} \binom{n}{j}(-1)^{n-j-1}(n-j)g^{n-j-1}(x)(g^j)^{(k)}(x) + T_{n,k+1}(x).$$

Note now that $(n-j)\binom{n}{j} = n\binom{n-1}{j}$. It follows that

$$\sum_{j=0}^{n} \binom{n}{j}(-1)^{n-j-1}(n-j)g^{n-j-1}(x)(g^j)^{(k)}(x) = \sum_{j=0}^{n-1} n\binom{n-1}{j}(-1)^{n-j-1}g^{n-j-1}(x)(g^j)^{(k)}(x) = nT_{n-1,k}(x).$$

Putting this together, we get the following key formula:

$$T'_{n,k}(x) = -ng'(x)T_{n-1,k}(x) + T_{n,k+1}(x).$$

i.e.

$$T_{n,k+1}(x) = ng'(x)T_{n-1,k}(x) + T'_{n,k}(x). \tag{1}$$

This formula positions us well to use induction.

When $k = 0$, we have

$$T_{n,0}(x) = \sum_{j=0}^{n} \binom{n}{j}(-1)^{n-j}g^{n-j}(x)g^j(x) = (g(x) - g(x))^n = 0$$

(we used the binomial formula). This shows that a) is true for $k = 0$. Suppose a) holds for some k and all $n > k$. If $n > k + 1$, then $n > k$ and $n - 1 > k$, so our assumption tells us that $T_{n,k}(x) = 0$ and $T_{n-1,k}(x) = 0$. By (1), we have $T_{n,k+1}(x) = 0$. Thus a) is true for all $n > k$ by induction.

We can now use a) to answer b). Note that when $n = k + 1$ the formula (1) and a) tell us that

$$T_{n,n}(x) = ng'(x)T_{n-1,n-1}(x) + T'_{n,n-1}(x) = ng'(x)T_{n-1,n-1}(x).$$

Since $T_{0,0}(x) = 1$, a straightforward induction tells us that

$$T_{n,n}(x) = n!(g'(x))^n.$$

Remark. The recursive formula (1) can also be obtained using the ideas from the first solution. Indeed, recall that if $H(u, w)$ is a differentiable function of two variables and $p(x)$, $q(x)$ are differentiable then

$$\frac{d}{dx}H(p(x), q(x)) = \frac{\partial}{\partial u}H(p(x), q(x))p'(x) + \frac{\partial}{\partial w}H(p(x), q(x))q'(x). \tag{2}$$

Let $F(u, w) = (g(u) - g(w))^n$ and $H(u, w) = \frac{\partial^k}{\partial u^k}F(u, w)$. In our first solution we showed that $T_{n,k}(x) = H(x, x)$. Using (2) with $p(x) = x = q(x)$ we get

$$T'_{n,k}(x) = \frac{\partial}{\partial u}H(x, x) + \frac{\partial}{\partial w}H(x, x).$$

Recall that $H(u, w) = \frac{\partial^k}{\partial u^k}F(u, w)$, so

$$T'_{n,k}(x) = \frac{\partial^{k+1}}{\partial u^{k+1}}F(x, x) + \frac{\partial}{\partial w}\frac{\partial^k}{\partial u^k}F(x, x) = T_{n,k+1}(x) + \frac{\partial^k}{\partial u^k}\frac{\partial}{\partial w}F(x, x).$$

Now

$$\frac{\partial}{\partial w}F(u,w) = -ng'(w)(g(u)-g(w))^{n-1}$$

so

$$\frac{\partial^k}{\partial u^k}\frac{\partial}{\partial w}F(u,w) = -ng'(w)\frac{\partial^k}{\partial u^k}(g(u)-g(w))^{n-1}$$

and

$$\frac{\partial^k}{\partial u^k}\frac{\partial}{\partial w}F(x,x) = -ng'(x)T_{n-1,k}(x).$$

This completes the derivation of (1).

Using the result of the problem and (1), it is not hard to prove the following beautiful formula due to Reinhold Hoppe:

Exercise. Let f, g be smooth functions. Prove that for any $k \geq 0$ we have

$$(f\circ g)^{(k)}(x) = \sum_{n=0}^{k} \frac{f^{(n)}(g(x))}{n!}T_{n,k}(x),$$

where $T_{n,k}$ are defined in the problem above (and depend only on g).

This explains our interest in the functions $T_{n,k}$ when $n < k$ (our problem was concerned with the case when $n \geq k$). One can wonder if there is any nice formula for $T_{n,k}(x)$ when $n < k$.

Exercise. Prove that

$$T_{n,k}(x) = k!\sum \binom{n}{a_1, a_2, \ldots, a_k}\prod_{j=1}^{k}\left(\frac{g^{(j)}(x)}{j!}\right)^{a_j},$$

where the summation on the right is over all possible choices of non-negative integers $a_1, \ldots, a_k$ such that $a_1 + 2a_2 + \ldots + ka_k = k$ and $a_1 + a_2 + \ldots + a_k = n$. Here the multinomial coefficient $\binom{n}{a_1,a_2,\ldots,a_k}$ is defined for any non-negative integers $a_1, \ldots, a_k$ such that $a_1 + \ldots + a_k = n$ by

$$\binom{n}{a_1, a_2, \ldots, a_k} = \frac{n!}{a_1!a_2!\ldots a_k!}.$$

Combining the last two exercises we get the following very nice formula:

$$\frac{(f\circ g)^{(k)}(x)}{k!} = \sum \frac{f^{(a_1+\ldots+a_k)}(g(x))}{(a_1+\ldots+a_k)!}\binom{a_1+\ldots+a_k}{a_1, a_2, \ldots, a_k}\prod_{j=1}^{k}\left(\frac{g^{(j)}(x)}{j!}\right)^{a_j},$$

where the summation on the right is over all possible choices of non-negative integers $a_1, \ldots, a_k$ such that $a_1 + 2a_2 + \ldots + ka_k = k$. This formula is often attributed to Francesco Faá di Bruno (around 1855), though it was apparently stated 50 years earlier by the French mathematician Louis Francois Antoine Arbogast.