# Mathematics 373 Workshop 7 Solutions

## Summation

## Fall 2003

**Introduction.** In this workshop, the Euler-Maclaurin summation formula will be derived. We have seen that formulas can be derived for a standard interval which is then rescaled to apply to other intervals. We follow D. E. Knuth, "The Art of Computer Programming, Volume 1, Fundamental Algorithms", Addison-Wesley, 1968, section 1.2.11.2.

**Problem 1.** We seek to compare

$$\sum_{k=1}^{n-1} f(k) \quad \text{and} \quad \int_1^n f(x)\,dx.$$

**1a Statement.** On the interval $k \le x \le k+1$, use the formula

$$\frac{d}{dx}\big((x-k-0.5)\,f(x)\big) = f(x) + (x-k-0.5)\,f'(x)$$

to obtain

$$\frac{1}{2}f(1) + \sum_{k=2}^{n-1} f(k) + \frac{1}{2}f(n) = \int_1^n f(x)\,dx + \int_1^n S_1(x)\,f'(x)\,dx,$$

where $S_1(x)$ is the "sawtooth function" that is given by $S_1(x) = x-k-0.5$ when $k \le x \le k+1$. (Its values at the integers are irrelevant, since it is only going to be integrated.)

**1a Solution.** For each $k$ with $1 \le k \le n-1$,

$$\begin{aligned}\int_k^{k+1} \frac{d}{dx}\big((x-k-0.5)\,f(x)\big)\,dx &= [(x-k-0.5)\,f(x)]_k^{k+1} \\ &= \big(0.5\,f(k+1)\big) - \big(-0.5\,f(k)\big) \\ &= 0.5\big(f(k+1) + f(k)\big)\end{aligned}$$

and

$$\int_k^{k+1} f(x) + (x-k-0.5)\,f'(x)\,dx = \int_k^{k+1} f(x)\,dx + \int_k^{k+1} S_1(x)\,f'(x)\,dx$$

Adding these causes $f(1)$ and $f(n)$ to retain their coefficients of 0.5 while the remaining $f(k)$ have **two** coefficients of 0.5 that combine to give a coefficient of 1. The sum of integrals of a single function over intervals that partition a big interval is just the integral over the big interval.

A close examination of this argument shows that it requires $n \ge 3$ for the sum of $f(k)$ to contain any terms. It is customary to extend this to $n = 2$ by claiming that a sum from 2 to 1 is an **empty sum** that has the value zero. One must be careful with this argument, since it is a useful convention only when summing over a set that has an **efficient** description as an empty set. That is, given numbers $a_k$ defined for $k > 0$, the numbers $A_n$ for $n \geq 0$ given by

$$A_n = \sum_{k=1}^{n} a_k$$

satisfy the **inductive definition**

$$A_0 = 0; \quad \text{and} \quad A_k = A_{k-1} + a_k \text{ for } k > 0.$$

This inductive definition leads to rigorous proofs of statements about sums that do not require visualizing expressions with **arbitrarily many** terms. If $a_k$ is defined for **all** integers, this inductive definition also gives a value to the sum when $n$ is negative, but this value does not agree with the usual interpretation of summation notation.

**1b Statement.** Continue this process by finding a function $S_2(x)$ such that $S_2'(x) = S_1(x)$. Note that

$$\int_k^{k+1} S_1(x)\,dx = 0$$

for all $k$ so that $S_2(x)$ can be chosen to be continuous (although it will fail to be differentiable at integer values of $x$). Also, $S_2(x+1) = S_2(x)$.

**1b Solution.** On the interval $[k, k+1]$, $S_1(x) = x - k - 0.5$, so, for $k \leq x \leq k+1$,

$$\int_k^x S_1(u)\,du = \int_k^x u - k - 0.5\,du = 0.5(x-k)^2 - 0.5(x-k)$$

since this is a function whose derivative is $S_1(x)$ and whose value at $x = k$ is zero. The value of this function at $x = k+1$ is also zero.

Any functions with derivative $S_1(x)$ must differ from this by a constant on $[k, k+1]$, so it will have the same value at $x = k+1$ as it has at $x = k$. The value of the integral at $x = k+1$ obtained from the interval $[k, k+1]$ is used to determine the constant term on the interval $[k+1, k+2]$. As long as the function is expressed in terms of powers of the **fractional part** of $x$, the constant terms will be the same on each interval.

Alternatively, one could write $S_2(x) = 0.5\big(S_1(x)\big)^2 + C$. Since $S_1(x+1) = S_1(x)$, the same is true for $S_2$. The graph of $S_2(x)$ consists of upward facing parabolic arcs with minima at the values $k + 0.5$ for all integers $k$.

Once $S_2(x)$ is written as a function of $S_1(x)$, or the **fractional part** of $x$ (which is $x-k$ for $k \leq x < k+1$), the periodicity is assured once continuity at integers is established.

**1c Statement.** The function $S_2(x)$ is only determined up to an additive constant. In order to be able to continue, this constant should be chosen so that

$$\int_k^{k+1} S_2(x)\,dx = 0$$

for all $k$. Find a choice of $S_2(x)$ with this property. Then

$$\frac{d}{dx}\big(S_2(x)\,f'(x)\big) = S_1(x)\,f'(x) + S_2(x)\,f''(x),$$

so $\int_1^n S_1(x)\,f'(x)\,dx$ can be expressed as the sum of a constant multiple of $\big(f'(n) - f'(1)\big)$ and the negative of the integral of $S_2(x)\,f''(x)$.

**1c Solution.** Let's use $S_2(x) = 0.5\big(S_1(x)\big)^2 + C$. If we write $x = k + 0.5 + u$ when $k \le x \le k+1$, then $-0.5 \le u \le 0.5$ and

$$\int_k^{k+1} S_2(x)\,dx = \int_{-0.5}^{0.5} \frac{1}{2}u^2 + C\,du = \left[\frac{1}{6}u^3 + Cu\right]_{-0.5}^{0.5} = \frac{1}{24} + C.$$

In this form $C = -1/24$. It is customary to express the quantities arising in this process as polynomials in $x - k$, so if we write $v = x - k = u + 0.5$, then $u = v - 0.5$ and

$$\begin{aligned}
\frac{1}{2}u^2 - \frac{1}{24} &= \frac{1}{2}\left(v - \frac{1}{2}\right)^2 - \frac{1}{24} \\
&= \frac{1}{2}v^2 - \frac{1}{2}v + \frac{1}{8} - \frac{1}{24} \\
&= \frac{1}{2}v^2 - \frac{1}{2}v + \frac{1}{12} \\
&= \frac{1}{2}\left(v^2 - v + \frac{1}{6}\right)
\end{aligned}$$

In particular, $S_2(k) = 1/12$ for all integers $k$ and $S_2(x)$ is a continuous function. The integration formula mentioned in the statement is then

$$\int_1^n S_1(x)\,f'(x)\,dx + \int_1^n S_2(x)\,f''(x)\,dx = \big[S_2(x)\,f'(x)\big]_1^n = \frac{1}{12}\big(f'(n) - f'(1)\big)$$

or

$$\int_1^n S_1(x)\,f'(x)\,dx = \frac{1}{12}\big(f'(n) - f'(1)\big) - \int_1^n S_2(x)\,f''(x)\,dx$$

This is the traditional way of writing the result of **integration by parts**, which is the integral calculus equivalent of the **product rule** of differential calculus.

**Comment.** This process can be continued indefinitely to get an asymptotic series for the difference between an integral and its approximation by the **composite trapezoidal rule**.

Problem 2 begins on next page

**Problem 2.** Here, we will demonstrate that a particular formula satisfies the conditions that characterize the process of Problem 1. Consider the function and its Taylor series

$$\frac{x}{e^x - 1} = \sum_{k=0}^{\infty} \frac{B_k x^k}{k!}.$$

This will be taken as the **definition** of the numbers $B_k$.

**2a Statement.** Show that

$$B(x) = \frac{x}{2} + \frac{x}{e^x - 1}$$

is an **even function**, so that $B_1 = -1/2$ and $B_{2k+1} = 0$ for $k > 0$. (We have introduced a name not present originally to use in the solution.)

**2a Solution.** We need to show that $B(-x) = B(x)$, so we first form $B(-x)$ and simplify its description to allow it to be compared to $B(x)$.

$$\begin{aligned}
B(-x) &= \frac{-x}{2} + \frac{-x}{e^{-x} - 1} \\
&= -\frac{x}{2} - \frac{xe^x}{1 - e^x} \\
&= -\frac{x}{2} + \frac{xe^x}{e^x - 1} \\
&= -\frac{x}{2} + x\left(1 + \frac{1}{e^x - 1}\right) \\
&= -\frac{x}{2} + x + \frac{x}{e^x - 1} \\
&= \frac{x}{2} + \frac{x}{e^x - 1} \\
&= B(x)
\end{aligned}$$

**2b Statement.** Use

$$e^x \frac{x}{e^x - 1} = x\frac{e^x}{e^x - 1} = x\left(1 + \frac{1}{e^x - 1}\right)$$

to show that

$$\sum_k \binom{m}{k} B_k = B_m$$

for $m \neq 1$. What is the corresponding formula when $m = 1$? (The index of this equation was written as $n$ in the statement, but $n$ is reserved for the upper limit of the original integral, so it has been changed to $m$ here.)

**2b Solution.** Multiplying the Taylor series for $e^x$ and $x/\left(e^x-1\right)$ gives

$$\sum_j \frac{x^j}{j!}\cdot\sum_k \frac{B_k x^k}{k!} = \sum_{j,k}\frac{B_k x^{j+k}}{j!k!}$$

where $j$ and $k$ take all positive integer values. If we introduce a new variable $m = j+k$, the terms of the sum can be described using $m$ and $k$ with $j = m-k$. The condition that $j \geq 0$ requires that $0 \leq k \leq m$, so we should sum over **just these** $k$ before summing over all $m \geq 0$. The denominator $j!k! = k!(m-k)!$ suggests the denominator in the **binomial coefficient** $m$-choose-$k$, one notation for which appears in statement. This binomial coefficient is **defined to be** zero unless $0 \leq k \leq m$, so the range of summation need not be written. The series for $xe^x/\left(e^x-1\right)$ is

$$\sum_m \left(\sum_k \binom{m}{k} B_k\right)\frac{x^m}{m!}.$$

We were given that this is $x + x/\left(e^x-1\right)$, so the coefficient of $x^m/m!$ in these two series are the same. For $m \neq 1$, this is the desired result. For $m = 1$, this is

$$\sum_k \binom{m}{k} B_k = B_m + 1.$$

Expanding the sum, we get $B_0 + B_1 + 1$, which reduces to $B_0 = 1$. Note also that the case $m = 0$ expands to $B_0 = B_0$. In general, the sum on the left is $B_m$ plus the sum of terms with $k < m$, so this can be solved for $B_{m-1}$ in terms of the $B_k$ with smaller index.

**2c Statement.** Let

$$B_m(x) = \sum_k \binom{m}{k} B_k x^{m-k}.$$

(The domain of the sum is $0 \leq k \leq m$, but it need not be shown because the binomial coefficient is zero outside that interval.) Show that $B'_m(x) = m B_{m-1}(x)$.

**2c Solution.** The definition of $B_m(x)$ leads to

$$B'_m(x) = \sum (m-k)\binom{m}{k} B_k x^{m-k-1}$$

However,

$$(m-k)\binom{m}{k} = \frac{(m-k)(m!)}{k!(m-k)!} = \frac{(m!)}{k!(m-k-1)!} = m\frac{(m-1)!}{k!(m-k-1)!} = m\binom{m-1}{k}$$

This is the coefficient of $x^{m-k-1}$ in $m B_{m-1}(x)$, as required.

**Comment.** This can be used to show that $S_m(x) = B_m(x-k)/m!$ for $k \leq x < k+1$. In particular, part (c) shows that $S'_m(x) = S_{m-1}(x)$ and part (b) shows that $S_m(1) = S_m(0)$ for $m \neq 1$ for this definition. These are the two **defining properties** of $S_m(x)$ developed in problem 1.

End of workshop 7