The theoretical derivation process presented here is a continuation and supplementary explanation of Section 4 - Illustrative Example in the article.

For the first functional scenario: $T_1 := x \leq 0,\ D_1 := n = 0$

Let's take $x = -10$ as an example:

The actual execution path of the program is:

$$
\begin{gathered}
sum = 0 \\
n = 0 \\
\neg(sum < x)
\end{gathered}
$$

The backward derivation process of Hoare logic is as follows:

$$
\begin{gathered}
\{n = 0\} \\
\neg(sum < x) \\
\{\neg(sum < x) \wedge n = 0\} \\
n = 0 \\
\{\neg(sum < x) \wedge 0 = 0\} \\
sum = 0 \\
\{\neg(0 < x) \wedge 0 = 0\}
\end{gathered}
$$

The derived conjunction is:

$$
\begin{gathered}
T_1 := x \leq 0 \\
C_{-10} := \neg(0 < x) \\
D_1' := (0 = 0) \\
T_1 \wedge C_{-10} \Rightarrow D_1' := x \leq 0 \wedge \neg(0 < x) \Rightarrow (0 = 0)
\end{gathered}
$$

That is to prove $x \leq 0 \wedge \neg(0 < x) \Rightarrow (0 = 0)$ is a tautology, which is obviously true.

For the second functional scenario:

$$
T_2 := x > 0,\ D_2 := \frac{(n-1)^2 n^2}{4} < x \leq \frac{n^2(n+1)^2}{4}
$$

Let's take $x = 66$ as an example:

The actual execution path of the program is:

$$sum = 0$$
$$n = 0$$
$$sum < x$$
$$n = n + 1$$
$$sum = sum + n * n * n$$
$$sum < x$$
$$n = n + 1$$
$$sum = sum + n * n * n$$
$$sum < x$$
$$n = n + 1$$
$$sum = sum + n * n * n$$
$$sum < x$$
$$n = n + 1$$
$$sum = sum + n * n * n$$
$$\neg(sum < x)$$

The backward derivation process of Hoare logic is as follows:

$$\{\frac{(n-1)^2 * n^2}{4} < x \leq \frac{n^2 * (n+1)^2}{4}\}$$
$$\neg(sum < x)$$
$$\{\neg(sum < x) \wedge \frac{(n-1)^2 * n^2}{4} < x \ \leq \frac{n^2 * (n+1)^2}{4}\}$$
$$sum = sum + n * n * n$$
$$\{\neg(sum + n^3 < x) \wedge \frac{(n-1)^2 * n^2}{4} < x \leq \frac{n^2 * (n+1)^2}{4}\}$$
$$n = n + 1$$
$$\{\neg(sum + (n+1)^3 < x) \wedge \frac{(n)^2 * (n+1)^2}{4} < x \leq \frac{(n+1)^2 * (n+2)^2}{4}\}$$
$$sum < x$$
$$\{sum < x \wedge \neg(sum + (n+1)^3 < x) \wedge \frac{(n)^2 * (n+1)^2}{4} < x \leq \frac{(n+1)^2 * (n+2)^2}{4}\}$$
$$sum = sum + n * n * n$$
$$\{sum + n^3 < x \wedge \neg(sum + n^3 + (n+1)^3 < x) \wedge \frac{(n)^2 * (n+1)^2}{4} < x \leq \frac{(n+1)^2 * (n+2)^2}{4}\}$$
$$n = n + 1$$
$$\{sum + (n+1)^3 < x \wedge \neg(sum + (n+1)^3 + (n+2)^3 < x)$$
$$\wedge \frac{(n+1)^2 * (n+2)^2}{4} < x \leq \frac{(n+2)^2 * (n+3)^2}{4}\}$$
$$sum < x$$
$$\{sum < x \wedge sum + (n+1)^3 < x \wedge \neg(sum + (n+1)^3 + (n+2)^3 < x)$$
$$\wedge \frac{(n+1)^2 * (n+2)^2}{4} < x \leq \frac{(n+2)^2 * (n+3)^2}{4}\}$$
$$sum = sum + n * n * n$$

$$\{sum + n^3 < x \wedge sum + n^3 + (n+1)^3 < x \wedge \neg(sum + n^3 + (n+1)^3 + (n+2)^3 < x)$$
$$\wedge \frac{(n+1)^2 * (n+2)^2}{4} < x \leq \frac{(n+2)^2 * (n+3)^2}{4}\}$$
$$n = n + 1$$
$$\{sum + (n+1)^3 < x \wedge sum + (n+1)^3 + (n+2)^3 < x \wedge \neg(sum + (n+1)^3 + (n+2)^3 + (n+3)^3 < x)$$
$$\wedge \frac{(n+2)^2 * (n+3)^2}{4} < x \leq \frac{(n+3)^2 * (n+4)^2}{4}\}$$
$$sum < x$$
$$\{sum < x \wedge sum + (n+1)^3 < x \wedge sum + (n+1)^3 + (n+2)^3 < x \wedge$$
$$\neg(sum + (n+1)^3 + (n+2)^3 + (n+3)^3 < x) \wedge \frac{(n+2)^2 * (n+3)^2}{4} < x \leq \frac{(n+3)^2 * (n+4)^2}{4}\}$$
$$sum = sum + n * n * n$$
$$\{sum + n^3 < x \wedge sum + n^3 + (n+1)^3 < x \wedge sum + n^3 + (n+1)^3 + (n+2)^3 < x \wedge$$
$$\neg(sum + n^3 + (n+1)^3 + (n+2)^3 + (n+3)^3 < x) \wedge \frac{(n+2)^2 * (n+3)^2}{4} < x \leq \frac{(n+3)^2 * (n+4)^2}{4}\}$$
$$n = n + 1$$
$$\{sum + (n+1)^3 < x \wedge sum + (n+1)^3 + (n+2)^3 < x \wedge sum + (n+1)^3 + (n+2)^3 + (n+3)^3 < x \wedge$$
$$\neg(sum + (n+1)^3 + (n+2)^3 + (n+3)^3 + (n+4)^3 < x)$$
$$\wedge \frac{(n+3)^2 * (n+4)^2}{4} < x \leq \frac{(n+4)^2 * (n+5)^2}{4}\}$$
$$sum < x$$
$$\{sum < x \wedge sum + (n+1)^3 < x \wedge sum + (n+1)^3 + (n+2)^3 < x$$
$$\wedge sum + (n+1)^3 + (n+2)^3 + (n+3)^3 < x \wedge \neg(sum + (n+1)^3 + (n+2)^3 + (n+3)^3 + (n+4)^3 < x)$$
$$\wedge \frac{(n+3)^2 * (n+4)^2}{4} < x \leq \frac{(n+4)^2 * (n+5)^2}{4}\}$$
$$n = 0$$
$$\{sum < x \wedge sum + (1)^3 < x \wedge sum + (1)^3 + (2)^3 < x$$
$$\wedge sum + (1)^3 + (2)^3 + (3)^3 < x \wedge \neg(sum + (1)^3 + (2)^3 + (3)^3 + (4)^3 < x)$$
$$\wedge \frac{(3)^2 * (4)^2}{4} < x \leq \frac{(4)^2 * (5)^2}{4}\}$$
$$sum = 0$$
$$\{0 < x \wedge 0 + (1)^3 < x \wedge 0 + (1)^3 + (2)^3 < x$$
$$\wedge 0 + (1)^3 + (2)^3 + (3)^3 < x \wedge \neg(0 + (1)^3 + (2)^3 + (3)^3 + (4)^3 < x)$$
$$\wedge \frac{(3)^2 * (4)^2}{4} < x \leq \frac{(4)^2 * (5)^2}{4}\}$$

The derived conjunction is:

$$T_2 := x > 0$$
$$C_{(66)} := 36 < x \wedge \neg(100 < x)$$
$$D_2' := 36 < x \wedge x \leq 100$$
$$T_2 \wedge C_{(66)} \Rightarrow D_2' := x > 0 \wedge 36 < x \wedge \neg(100 < x) \Rightarrow 36 < x \wedge x \leq 100$$

To prove $T_2 \wedge C_{(66)} \Rightarrow D_2'$ is a tautology.

That is equivalent to proving that the formula $T_2 \wedge C_{(66)} \wedge \neg D_2'$ is unsatisfiable.

$$T_2 \wedge C_{(66)} \wedge \neg D_2' := x > 0 \wedge 36 < x \wedge \neg(100 < x) \wedge \neg(36 < x \wedge x \leq 100)$$

After solving with the Z3 Constraint Solver, it can be determined that the formula is unsatisfiable.

If we change the code $sum < x$ into $sum <= x$:

The derived conjunction will be:

$$T_2 \wedge C_{(66)} \wedge \neg D_2' := x > 0 \wedge 36 \leq x \wedge \neg(100 \leq x) \wedge \neg(36 < x \wedge x \leq 100)$$

which is satisfiable and Z3 will produce a counterexample x = 36.