Asymptotic Analysis of Functions

In order to analyze the efficiency of an algorithm, we consider its running time $t(n)$ as a function of the input size *n*. We look at large enough *n* such that only the order of growth of *t*(*n*) is relevant. In such asymptotic analysis, we are interested in whether the function scales as exponential (*e.g.*, 10^{*n*}), polynomial (*e.g.*, n^3) or logarithmic (*e.g.*, log₂*n*), for example. We use the following asymptotic notations.

 Θ **notation:** Given a function $g(n)$, $\Theta(g(n)) = \{f(n):$ there exist positive constants c_1 , c_2 and n_0 such that $c_1 g(n) \le f(n) \le c_2 g(n)$ for all $n \ge n_0$. We say $\Theta(g(n))$ is an *asymptotically tight bound* for $f(n)$.

(Example) In the molecular dynamics (MD) program, md.c, the computational bottleneck is the sum over all distinct atom pairs (*i*, *j*) to compute interatomic forces, implemented in a doublynested loop (see function *ComputeAccel*()):

$$
\begin{array}{l}\n\text{for } (i=0; i
$$

The running time of this loop is proportional to the total number of iterations,

$$
f(n) = 1 + 2 + \dots + (n - 1) = \frac{(n - 1)(1 + n - 1)}{2} = \frac{n^2 - n}{2},
$$

which is $\Theta(n^2)$.

(Proof)

Let us consider inequalities

$$
c_1 n^2 \le f(n) = \frac{n^2 - n}{2} \le c_2 n^2 \,. \tag{1}
$$

Dividing both sides by n^2 yields

$$
c_1 \le f(n) = \frac{1}{2} - \frac{1}{2n} \le c_2 \, .
$$

The right-hand inequality is satisfied for any positive *n* by choosing $c_2 \ge 1/2$. On the other hand, the left-hand inequality holds for all $n \ge 2$ if $c_1 \le 1/4$ (see the figure below). By choosing $c_1 = 1/4$, $c_2 = 1/2$ and $n_0 = 2$, Eq. (2) thus holds for all $n \ge n_0$. By definition, then $f(n)$ is $\Theta(n^2)$. //

O (or "big-oh") notation: Given a function $g(n)$, $O(g(n)) = {f(n)}$: there exist positive constants *c* and n_0 such that $f(n) \le cg(n)$ for all $n \ge n_0$. We say $O(g(n))$ is an *asymptotically upper bound* for $f(n)$. Note that $O(g(n))$ is a superset of $O(g(n))$. Outside computer science, the big-oh notation is most commonly used. While most bounds discussed in this class are tight bounds, we will loosely use the big-oh notation unless specific distinction is required.

References

- 1. A. Grama *et al*., *Introduction to Parallel Computing, Second Edition* (Addison Wesley, 2003), Appendix A.2—Order analysis of functions.
- 2. T. H. Cormen *et al*., *Introduction to Algorithms, Third Edition* (MIT Press, 2009), Chap. 3— Growth of functions.