Métodos Numéricos y Simulaciones en Astrofísica

Parte 1: Herramientas básicas y formatos numéricos

Experimento Computacional

Fenómeno físico

Modelo matemático

Aproximación algebraica

exactitud
eficiencia
estabilidad

Algoritmo numérico

Programa de simulación

Experimento computacional

Herramientas Básicas

Teorema de Taylor:

Theorem 1.1 *(Taylor's Theorem with Remainder)* *Let $f(x)$ have $n+1$ continuous derivatives on $[a,b]$ for some $n \geq 0$, and let $x, x_0 \in [a,b]$. Then*

$$f(x) = p_n(x) + R_n(x)$$

for

$$p_n(x) = \sum_{k=0}^{n} \frac{(x-x_0)^k}{k!} f^{(k)}(x_0) \tag{1.1}$$

and

$$R_n(x) = \frac{1}{n!} \int_{x_0}^{x} (x-t)^n f^{(n+1)}(t)\, dt. \tag{1.2}$$

Moreover, there exists a point ξ_x between x and x_0 such that

$$R_n(x) = \frac{(x-x_0)^{n+1}}{(n+1)!} f^{(n+1)}(\xi_x). \tag{1.3}$$

Herramientas Básicas

Serie de Taylor:

$$p_n(x) = \sum_{k=0}^{n} \frac{(x-x_0)^k}{k!} f^{(k)}(x_0)$$

$$e^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots + \frac{1}{n!}x^n + \frac{1}{(n+1)!}x^{n+1}e^{\xi_x}$$

$$= \sum_{k=0}^{n} \frac{1}{k!}x^k + R_n(x),$$

$x_0 = 0$

$$e^x = \frac{(x-0)^0}{0!}e^0 + \frac{(x-0)^1}{1!}e^0 + \frac{(x-0)^2}{2!}e^0 + \frac{(x-0)^3}{3!}e^0 + \ldots$$

Herramientas Básicas

Serie de Taylor: e^x

$x \in [-1,1]$

$$e^x = \underbrace{1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \cdots + \frac{1}{n!}x^n}_{p_n(x),\ \text{polynomial}} + \underbrace{\frac{1}{(n+1)!}x^{n+1}e^{c_x}}_{R_n(x),\ \text{remainder}},$$

$$|e^x - p_n(x)| = |R_n(x)| \leq 10^{-6}$$

$$\begin{aligned}
|R_n(x)| &= \frac{|x^{n+1}e^{c_x}|}{(n+1)!} = \frac{|x|^{n+1}e^{c_x}}{(n+1)!}, && \text{because } e^z > 0 \text{ for all } z \\
&\leq \frac{e^{c_x}}{(n+1)!}, && \text{because } |x| \leq 1 \text{ for all } x \in [-1,1] \\
&\leq \frac{e}{(n+1)!}, && \text{because } e^{c_x} \leq e \text{ for all } x \in [-1,1].
\end{aligned}$$

Puedo encontrar el valor de n

$$\frac{1}{(n+1)!}e \leq 10^{-6}$$

→

$$|e^x - p_n(x)| = |R_n(x)| \leq \frac{1}{(n+1)!}e \leq 10^{-6}$$

Herramientas Básicas

Serie de Taylor: e^x

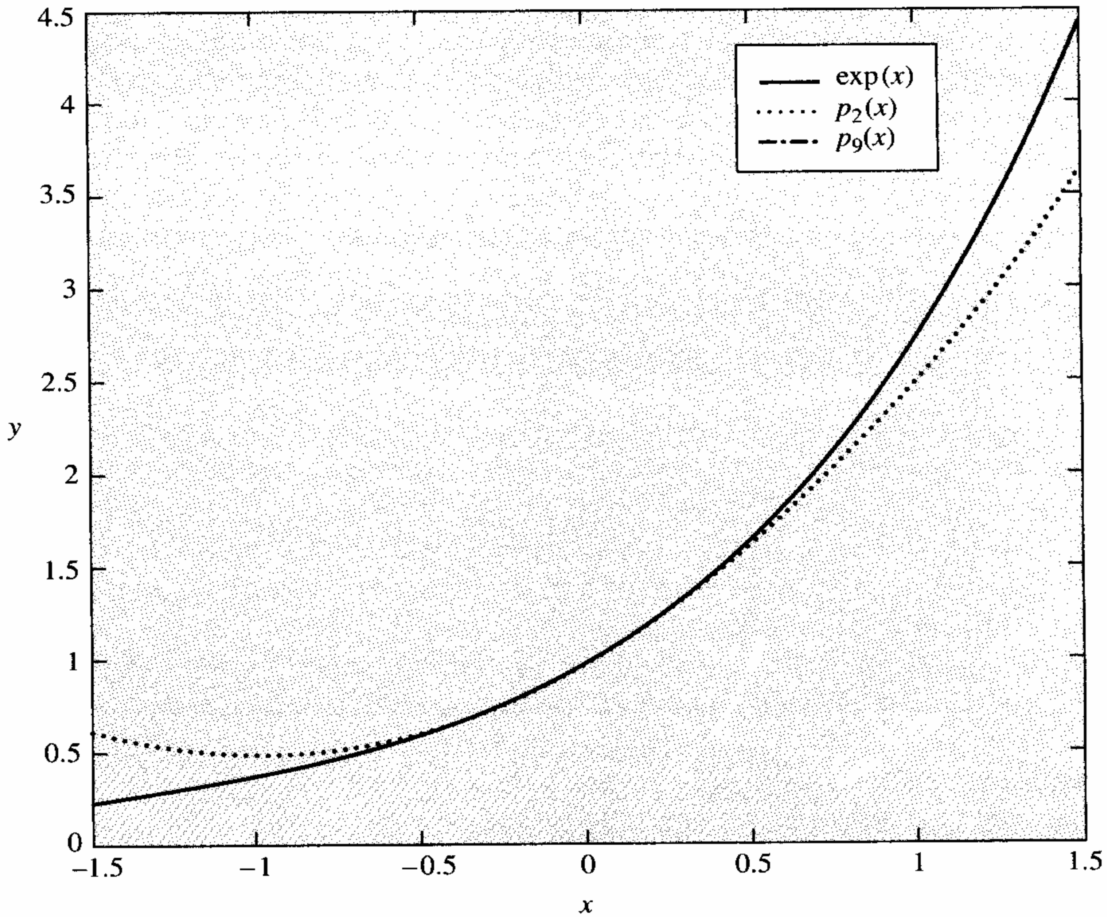


FIGURE 1.1 Taylor approximation: e^x, $p_9(x) \approx e^x$, and $p_2(x) \approx e^x$. Note that e^x and $p_9(x)$ are indistinguishable on this plot.

Herramientas Básicas

Serie de Taylor: e^x

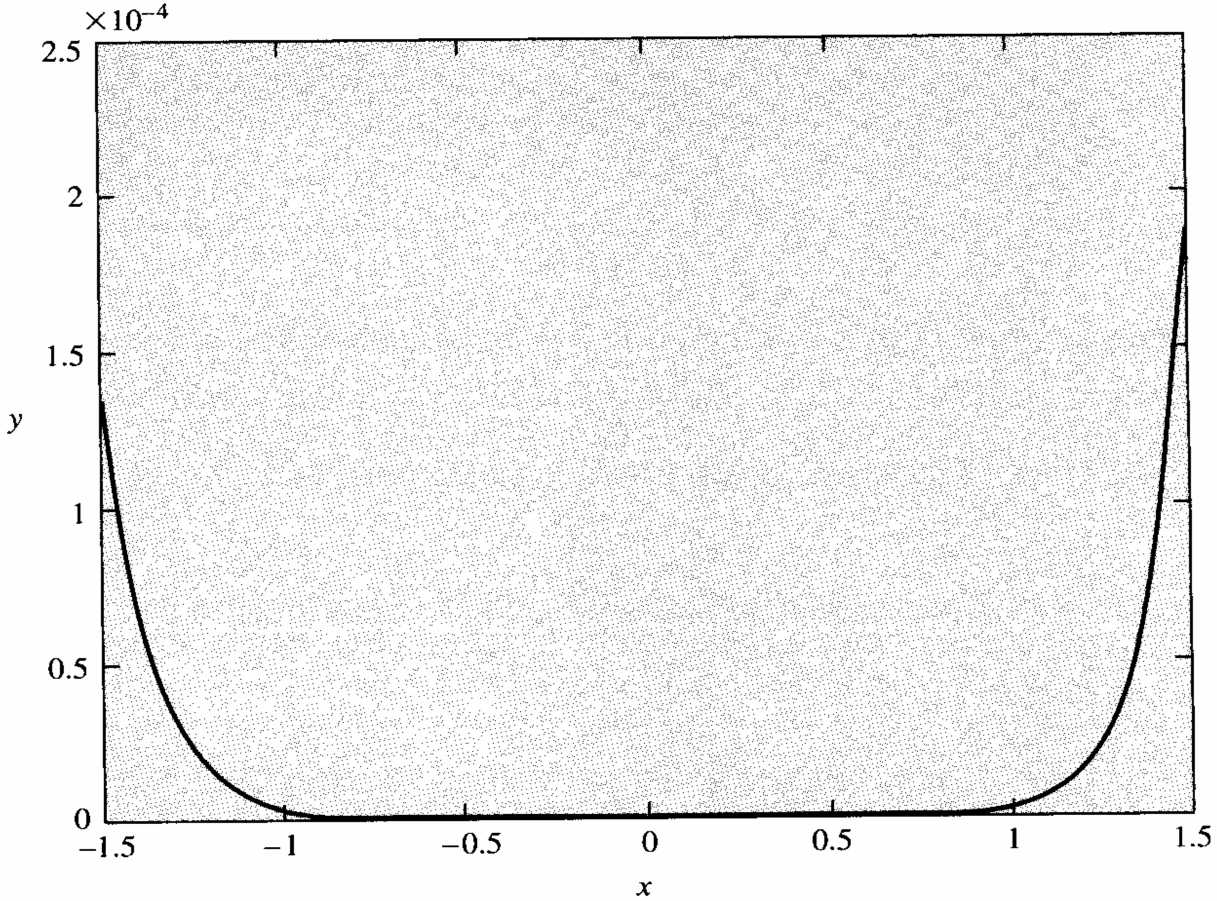


FIGURE 1.2 Error in Taylor approximation: $e^x - p_9(x)$.

Herramientas Básicas

Serie de Taylor:

Desarrollo de segundo orden para $f(x)=(x+1)^{1/2}$, para $x_0=0$

$$f(x_0) = f(0) = 1$$

$$f'(x) = \frac{1}{2}(x+1)^{-1/2} \quad \Rightarrow \quad f'(x_0) = \frac{1}{2}$$

$$f''(x) = -\frac{1}{2} \times \frac{1}{2}(x+1)^{-3/2} \quad \Rightarrow \quad f''(x_0) = -\frac{1}{4}$$

$$p_2(x) = f(x_0) + (x-x_0)f'(x_0) + \frac{1}{2}(x-x_0)^2 f''(x_0) = 1 + \frac{1}{2}x - \frac{1}{8}x^2.$$

$$|R_2(x)| = \left|\frac{1}{3!}(x-x_0)^3 f'''(\xi_x)\right|$$

$$= \frac{1}{6}|x|^3 \left|\frac{3}{2} \times \frac{1}{2} \times \frac{1}{2}(\xi_x+1)^{-5/2}\right|$$

$$= \frac{1}{16}|x|^3 |\xi_x + 1|^{-5/2}.$$

$$|\xi_x + 1|^{-5/2} \leq |0+1|^{-5/2} = 1,$$

$$|R_3(x)| \leq 1/16 = 0.0625, \text{ for all } x \in [0,1].$$

Herramientas Básicas

Serie de Taylor:

$$
\begin{aligned}
f(x+h) =& f(x) + ([x+h]-x)f'(x) + \frac{1}{2}([x+h]-x)^2 f''(x) \\
&+ \cdots + \frac{1}{n!}([x+h]-x)^n f^{(n)}(x) \\
&+ \frac{1}{(n+1)!}([x+h]-x)^{n+1} f^{(n+1)}(\xi) \\
=& f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \cdots + \frac{1}{n!}h^n f^{(n)}(x) \\
&+ \frac{1}{(n+1)!}h^{n+1} f^{(n+1)}(\xi).
\end{aligned}
$$

Teoremas del valor medio y otros

Theorem 1.2 (Mean Value Theorem) *Let f be a given function, continuous on $[a,b]$ and differentiable on (a,b). Then there exists a point $\xi \in [a,b]$ such that*

$$f'(\xi) = \frac{f(b) - f(a)}{b - a}. \tag{1.4}$$

Theorem 1.3 (Intermediate Value Theorem) *Let $f \in C([a,b])$ be given, and assume that W is a value between $f(a)$ and $f(b)$, i.e., either $f(a) \leq W \leq f(b)$, or $f(b) \leq W \leq f(a)$. Then there exists a point $c \in [a,b]$ such that $f(c) = W$.*

Theorem 1.4 (Extreme Value Theorem) *Let $f \in C([a,b])$ be given; then there exists a point $m \in [a,b]$ such that $f(m) \leq f(x)$ for all $x \in [a,b]$, and a point $M \in [a,b]$ such that $f(M) \geq f(x)$ for all $x \in [a,b]$. Morever, f achieves its maximum and minimum values on $[a,b]$ either at the endpoints a and b, or at a critical point.*

Teoremas del valor medio y otros

Theorem 1.5 (Integral Mean Value Theorem) *Let f and g both be in $C([a,b])$, and assume further that g does not change sign on $[a,b]$. Then there exists a point $\xi \in [a,b]$ such that*

$$\int_a^b g(t)f(t)dt = f(\xi)\int_a^b g(t)\,dt. \tag{1.5}$$

Theorem 1.6 (Discrete Average Value Theorem) *Let $f \in C([a,b])$ and consider the sum*

$$S = \sum_{k=1}^{n} a_k f(x_k),$$

where each point $x_k \in [a,b]$, and the coefficients satisfy

$$a_k \geq 0, \qquad \sum_{k=1}^{n} a_k = 1.$$

Then there exists a point $\eta \in [a,b]$ such that $f(\eta) = S$, i.e.,

$$f(\eta) = \sum_{k=1}^{n} a_k f(x_k).$$

Error y Aproximación

- A : una cantidad que queremos calcular
- A_h: una aproximación a esa cantidad

$$\text{error} = A - A_h;$$

$$\text{absolute error} = |A - A_h|;$$

$$\text{relative error} = \frac{|A - A_h|}{|A|},$$

- El error relativo es una buena medicion.
- Estos errores son errores de computación.

Error y Aproximación

- Aproximación

$$\lim_{h \to 0} A_h = A \quad \Rightarrow \quad A_h \approx A$$

- Es una relación de equivalencia y satisface las siguientes propiedades:
  - Transitiva :
  - Simétrica :
  - Reflexiva :

$$A \approx B, \quad B \approx C \quad \Rightarrow \quad A \approx C,$$
$$A \approx B \quad \Rightarrow \quad B \approx A,$$
$$A \approx A.$$

Notación: Orden Asintótico

Definition 1.1 (Asymptotic Order Notation) *For a given value y, let $\{y_h\}$ be a set of values parameterized by h, which we assume is small, such that $y_h \approx y$ for small h. If there exists a positive function $\beta(h)$, $\beta(h) \to 0$ as $h \to 0$, and a constant $C > 0$, such that for all h sufficiently small,*

$$|y - y_h| \leq C\beta(h),$$

then we say that

$$y = y_h + O(\beta(h)).$$

Similarly, if $\{y_n\}$ is a set of values parameterized by n, which we assume is large, such that $y_n \approx y$ for large n, and if there exists a positive function $\beta(n)$, $\beta(n) \to 0$ as $n \to \infty$, and a constant $C > 0$, such that for all n sufficiently large,

$$|y - y_n| \leq C\beta(n),$$

then we say that

$$y = y_n + O(\beta(n)).$$

Notación: Orden Asintótico

- Ejemplo: sea

$$A = \int_0^\infty e^{-2x}\, dx$$
$$A_n = \int_0^n e^{-2x}\, dx.$$

- Es simple demostrar que:

$$A = \tfrac{1}{2} \text{ and } A_n = \tfrac{1}{2} - \tfrac{1}{2}e^{-2n},$$

- Entonces: $$A = A_n + O(e^{-2n}).$$

- Donde: $$\beta(n) = e^{-2n}.$$

Notación: Orden Asintótico

Theorem 1.7 *Let* $y = y_h + O(\beta(h))$ *and* $z = z_h + O(\gamma(h))$, *with* $b\beta(h) > \gamma(h)$ *for all* h *near zero. Then*

$$y + z = y_h + z_h + O(\beta(h) + \gamma(h))$$
$$y + z = y_h + z_h + O(\beta(h))$$
$$Ay = Ay_h + O(\beta(h)).$$

In the last equation, A *is an arbitrary constant, independent of* h.

Notación: Orden Asintótico

We close this section with a simple example that illustrates the utility of the O notation. Consider the combination of function values

$$D = -f(x+2h) + 4f(x+h) - 3f(x),$$

where f is assumed to be continuous and smooth, and h is a (small) parameter. We can use Taylor's Theorem, together with the definition of the O notation, to write

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + O(h^3)$$

and

$$f(x+2h) = f(x) + 2hf'(x) + 2h^2 f''(x) + O(h^3).$$

Notación: Orden Asintótico

Therefore,

$$\begin{aligned}
D &= -f(x+2h) + 4f(x+h) - 3f(x) \\
&= -\left(f(x) + 2hf'(x) + 2h^2 f''(x) + O(h^3)\right) \\
&\quad + 4\left(f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + O(h^3)\right) - 3f(x) \\
&= (-1+4-3)f(x) + (-2h+4h)f'(x) + (-2h^2+2h^2)f''(x) + O(h^3) \\
&= 2hf'(x) + O(h^3).
\end{aligned}$$

If we then solve this for $f'(x)$, we get

$$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + O(h^2),$$

where we have used the fact that $O(h^3)/h = O(h^2)$ (see Exercise 10); thus we can use the expression on the right as an approximation to the derivative, and the remainder will be bounded by a constant times h^2. See Sections 2.2 and 4.5 for more on approximations to the derivative. This particular approximation is derived again, by alternate means, in Section 4.5. ■

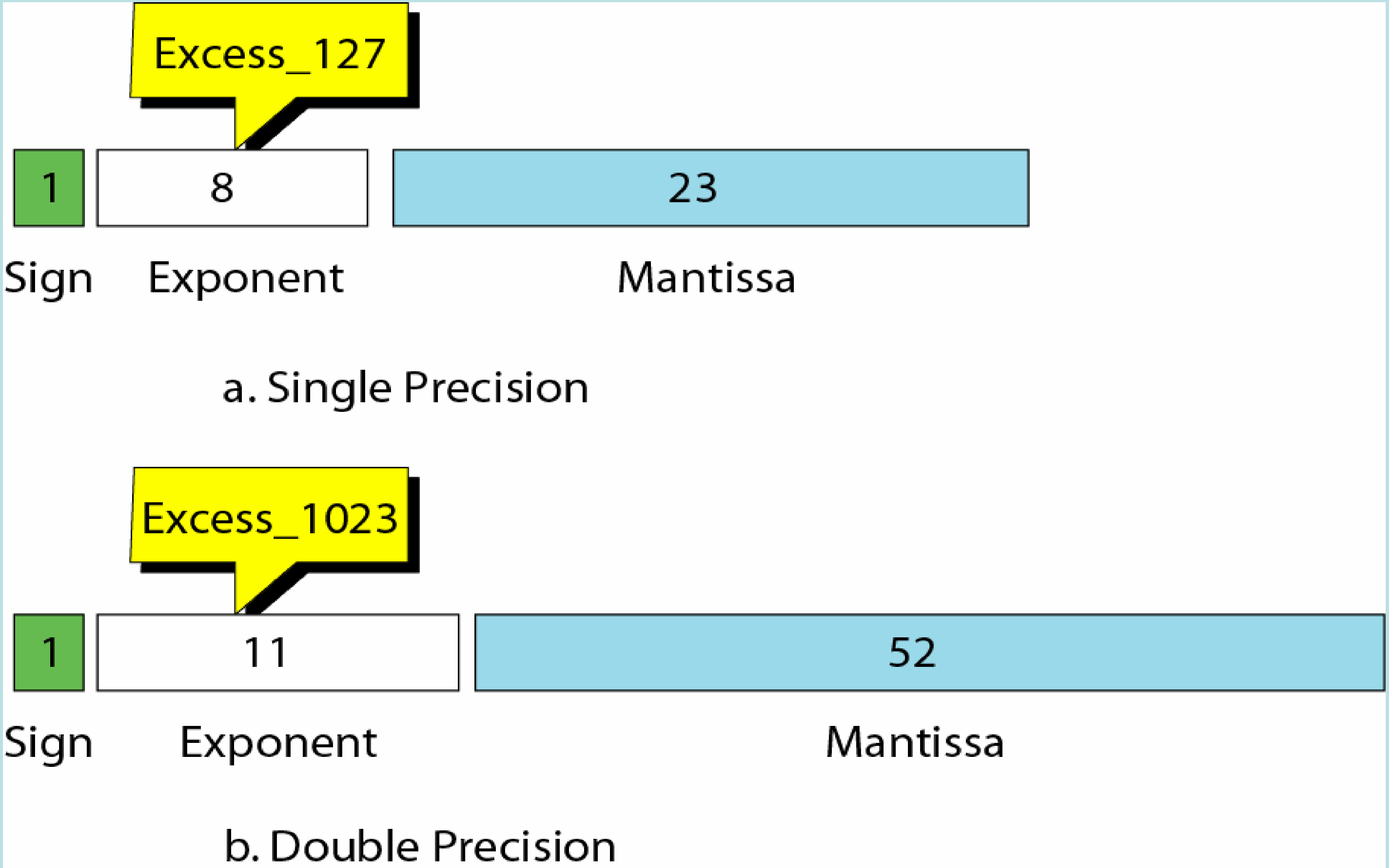
Aritmética Computacional

- La aritmética computacional es generalmente inexacta!
  - Los errores pueden ser pequeños pero se pueden acumular y dominar el resultado.
  - Ejemplo: aritmética de punto flotante
    - Reference: An Introduction to Computer Science, Chapter 3, Excess System (Excess_127 or Excess_1023)

$$x = \sigma \times f \times \beta^{t-p}.$$

σ	t	f

Aritmética Computacional



Errores de redondeo y truncamiento

$$x = 0.1, \qquad y = 0.00003,$$

$$z = x + y = 0.10003.$$

$$\begin{aligned}\tilde{x} &= 0.00011001 \quad 10011001 \quad 10011001 \quad 100_2\\ &= 0.0999999940395\ldots\end{aligned}$$

$$\begin{aligned}\tilde{y} &= 0.00000000 \quad 00000001 \quad 11110111 \quad 01010001 \quad 0000010_2\\ &= 0.0000299999992421\ldots\end{aligned}$$

- Error de redondeo: $E_r = 0.5 \times 10^{-8}$
- Error de truncamiento: $E_t = 0.7 \times 10^{-8}$

Cancelación por Resta

- Si a y b son exactos hasta 16 dígitos decimales. La diferencia $c = a - b$ mantiene esa exactitud?
- Ejemplo:

$$a = 0.9999000049998333$$
$$b = 0.9999990000005000$$
$$c = -0.0000989950006667.$$

El resultado c es exacto hasta 12 dígitos solamente (para la aritmética computacional!)

- Esto se debe a que estamos restando dos números casi iguales.