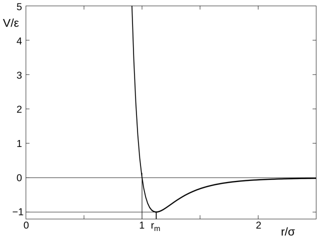
Taylor Polynomials



$$V(r) = \varepsilon \left[\left(\frac{r_m}{r} \right)^{12} - 2 \left(\frac{r_m}{r} \right)^{6} \right]$$

"Lennard-Jones potential"

- what is the equilibrium separation r? $r = r_m$
- what happens if r is changed slightly from $r = r_m$?
- how might you estimate the frequency at which it will vibrate?
  approximate the graph of $V(r)$ near $r = r_m$ by a parabola, which generates "simple harmonic motion".

Goal for today: find the polynomial of given degree which "best" approximates a function $f(x)$ "near" a point $x = a$.

Taylor Polynomials

- the **constant** function best approximating $f(x)$ near $x = a$ is:
  $T_0(x) = f(a)$

- the **linear** function best approximating $f(x)$ near $x = a$ is:
  $T_1(x) = L(x) = f(a) + f'(a)(x - a)$,

our old friend! In what sense is it the "best" linear approximation?

$T_1(a) = f(a)$ and $T_1'(a) = f'(a)$ (gets value *and* slope right at a)

- what **quadratic** function best approximates f near $x = a$?

$T_2(x) = c_2(x-a)^2 + c_1(x-a) + c_0$, and we require:

$$f(a) = T_2(a) = c_0$$
$$f'(a) = T_2'(a) = (2c_2(x-a) + c_1)|_{x=a} = c_1$$
$$f''(a) = T_2''(a) = 2c_2 \implies c_2 = \frac{1}{2}f''(a)$$

$$\implies T_2(x) = f(a) + f'(a)(x-a) + \frac{1}{2}f''(a)(x-a)^2 .$$

Taylor Polynomials

- which **cubic** polynomial best approximates f near $x = a$?

$T_3(x) = c_3(x-a)^3 + c_2(x-a)^2 + c_1(x-a) + c_0$, and we require:

$$f(a) = T_3(a) = c_0$$
$$f'(a) = T_3'(a) = (3c_2(x-a)^2 + 2c_2(x-a) + c_1)|_{x=a} = c_1$$
$$f''(a) = T_3''(a) = 6c_3(x-a) + 2c_2 \implies c_2 = \tfrac{1}{2}f''(a)$$
$$f'''(a) = T_3'''(a) = 6c_3 \implies c_3 = \tfrac{1}{6}f'''(a)$$

$$T_3(x) = f(a) + f'(a)(x-a) + \tfrac{1}{2}f''(a)(x-a)^2 + \tfrac{1}{6}f'''(a)(x-a)^3 \ .$$

- the polynomial of degree n which best approximates f near a is

The n-th order Taylor polynomial for f about $x = a$:

$$T_n(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n$$

– *factorial*: $n! = n(n-1)(n-2)\cdots(2)(1)$

– *n-th derivative*: $f^{(3)}(a) = f'''(a)$, $f^{(4)}(a) = f''''(a)$, etc.

– *can check*: $T_n(a) = f(a)$, $T_n'(a) = f'(a)$, ..., $T_n^{(n)}(a) = f^{(n)}(a)$.

Taylor Polynomials

Example: Find the third order **Maclaurin polynomial** (Taylor poly. centred at $a = 0$) for $\sin(x)$. Use it to approximate $\sin(1/4)$.

$f(x) = \sin(x), \;\; f'(x) = \cos(x), \;\; f''(x) = -\sin(x), \;\; f'''(x) = -\cos(x)$
$f(0) = 0, \;\; f'(0) = 1, \;\; f''(0) = 0, \;\; f'''(0) = -1$

$$\implies \quad T_3(x) = f(0) + f'(0)x + \frac{f''(0)}{2}x^2 + \frac{f'''(0)}{6}x^3 = \boxed{x - \frac{1}{6}x^3}.$$

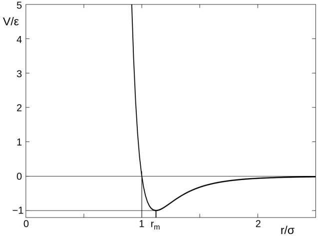
$\sin(1/4) \approx T_3(1/4) = \frac{1}{4} - \frac{1}{6}\frac{1}{4^3} = \frac{95}{384}$

(calculator: $\sin(1/4) \approx 0.247404$ while $\frac{95}{384} \approx 0.247396$)

Example: Find Maclaurin polynomials (as many terms as you can – try to find a pattern) for: 1. $\sin(x)$ 2. $\cos(x)$ 3. e^x 4. $\frac{1}{1-x}$

1. $\sin(x) \approx x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 - \frac{1}{7!}x^7 + \cdots$
2. $\cos(x) \approx 1 - \frac{1}{2}x^2 + \frac{1}{4!}x^4 - \frac{1}{6!}x^6 - \cdots$
3. $e^x \approx 1 + x + \frac{1}{2}x^2 + \frac{1}{3!}x^3 + \frac{1}{4!}x^4$
4. $\frac{1}{1-x} \approx 1 + x + x^2 + x^3 + x^4 + \cdots$

Taylor Polynomials



$$V(r) = \varepsilon\left[\left(\frac{r_m}{r}\right)^{12} - 2\left(\frac{r_m}{r}\right)^{6}\right]$$

"Lennard-Jones potential"

What is the frequency of small vibrations of r near r_{min}?

- find the second-order Taylor polynomial for $V(r)$ at $r = r_m$:

$V'(r) = \frac{\varepsilon}{r_m}\left[-12\left(\frac{r_m}{r}\right)^{13} + 12\left(\frac{r_m}{r}\right)^{7}\right]$, so $V'(r_m) = 0$ (of course!)

$V''(r) = 12\frac{\varepsilon}{r_m^2}\left[13\left(\frac{r_m}{r}\right)^{14} - 7\left(\frac{r_m}{r}\right)^{8}\right]$, so $V''(r_m) = 72\frac{\varepsilon}{r_m^2}$

$$V(r) \approx T_2(r) = V(r_m) + V'(r_m)(r - r_m) + \frac{1}{2}V''(r_m)(r - r_m)^2$$

$$= \boxed{-\varepsilon + 36\frac{\varepsilon}{r_m^2}(r - r_m)^2}$$

- Newton, for $\tilde{r} = r - r_m$: $\frac{d^2\tilde{r}}{dt^2} = -\frac{1}{m}V'(r) \approx -\frac{72\varepsilon}{m r_m^2}\tilde{r}$

so $\tilde{r}(t) \approx A\sin(kt) + B\cos(kt)$ with frequency $\boxed{k = \sqrt{\frac{72\varepsilon}{m r_m^2}}}$

Taylor Polynomials: Size of the Error

Recall: our error formula for the linear approximation

$f(x) \approx L(x) = T_1(x) = f(a) + f'(a)(x-a)$:

$$f(x) - T_1(x) = \frac{1}{2} f''(c)(x-a)^2$$

for some c between a and x. This generalizes to:

$$f(x) - T_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(c)(x-a)^{n+1}$$

for some c between a and x.

Example: give a rough estimate of the error in
$\sin(\frac{1}{4}) \approx T_3(\frac{1}{4}) = \frac{1}{4} - \frac{1}{6}(\frac{1}{4})^3 = \frac{95}{384}$

- error $= \sin(\frac{1}{4}) - T_3(\frac{1}{4}) = \frac{1}{4!} f^{(4)}(c)(\frac{1}{4})^4$, for some $0 < c < \frac{1}{4}$
- $f(x) = \sin(x)$, $f^{(4)}(x) = \sin(x)$, so: $0 < f^{(4)}(c) < 1$
- $\implies 0 <$ error $< \frac{1}{24}(\frac{1}{4})^4 \approx 0.00016$ (true error: 0.000008)

Indeterminate Forms and L'Hôpital's Rule

Example: Evaluate (in several different ways):

$$\lim_{x\to 0} \frac{x\sin(x)}{1-\cos(x)}.$$

- Taylor: $\lim_{x\to 0} \frac{x\sin(x)}{1-\cos(x)} = \lim_{x\to 0} \frac{x(x-\frac{1}{6}x^3+\cdots)}{1-(1-\frac{1}{2}x^2+\frac{1}{24}x^4+\cdots)}$
  $= \lim_{x\to 0} \frac{x^2-\frac{1}{6}x^4+\cdots}{\frac{1}{2}x^2-\frac{1}{24}x^4+\cdots} = \lim_{x\to 0} \frac{1-\frac{1}{6}x^2+\cdots}{\frac{1}{2}-\frac{1}{24}x^4+\cdots} = \frac{1}{\frac{1}{2}} = 2$

- $\lim_{x\to 0} \frac{x\sin(x)}{1-\cos(x)} = \lim_{x\to 0} \frac{x\sin(x)}{1-\cos(x)} \frac{1+\cos(x)}{1+\cos(x)}$
  $= \lim_{x\to 0} \frac{x\sin(x)(1+\cos(x))}{1-\cos^2(x)} = \lim_{x\to 0} \frac{x\sin(x)(1+\cos(x))}{\sin^2(x)}$
  $= \lim_{x\to 0} \left[\frac{x}{\sin(x)}\right] \lim_{x\to 0} (1+\cos(x)) = 1\cdot 2 = 2$

- l'Hôpital: $\lim_{x\to 0} \frac{x\sin(x)}{1-\cos(x)} = \lim_{x\to 0} \frac{\frac{d}{dx}(x\sin(x))}{\frac{d}{dx}(1-\cos(x))}$
  $= \lim_{x\to 0} \frac{\sin(x)-x\cos(x)}{\sin(x)} = \lim_{x\to 0} \frac{\frac{d}{dx}(\sin(x)+x\cos(x))}{\frac{d}{dx}\sin(x)}$
  $= \lim_{x\to 0} \frac{2\cos(x)+x\sin(x)}{\cos(x)} = \frac{2}{1} = 2$

Theorem: (**L'Hôpital's rule**) Let f and g be differentiable functions for x near a, with $g'(x) \neq 0$ there (except possibly at $x = a$). If $\lim_{x\to a} f(x) = \lim_{x\to a} g(x) = 0$ (or ∞ or $-\infty$), then

$$\lim_{x\to a} \frac{f(x)}{g(x)} = \lim_{x\to a} \frac{f'(x)}{g'(x)}$$

if this limit exists, or is $\pm\infty$.

A rigorous proof can be given using the Mean Value Theorem (next topic), but we can easily demonstrate the idea using Taylor approximation: if $f(a) = g(a) = 0$, then

$$f(x) = f'(a)(x-a) + \tfrac{1}{2}(x-a)^2 + \cdots$$
$$g(x) = g'(a)(x-a) + \tfrac{1}{2}(x-a)^2 + \cdots,$$

$$\lim_{x\to a} \tfrac{f(x)}{g(x)} = \lim_{x\to a} \tfrac{f'(a)(x-a)+\frac{1}{2}(x-a)^2+\cdots}{g'(a)(x-a)+\frac{1}{2}(x-a)^2+\cdots}$$
$$= \lim_{x\to a} \tfrac{f'(a)+\frac{1}{2}(x-a)+\cdots}{g'(a)+\frac{1}{2}(x-a)+\cdots} = \tfrac{f'(a)}{g'(a)} \quad (\text{if } g'(a) \neq 0)$$

Indeterminate Forms and L'Hôpital's Rule

Example: $\lim\limits_{x\to 0} \frac{2-x^2-2\cos(x)}{x^3}$
$= \lim\limits_{x\to 0} \frac{-2x+2\sin(x)}{3x^2} = \lim\limits_{x\to 0} \frac{-2+2\cos(x)}{6x} = \lim\limits_{x\to 0} \frac{-2\sin(x)}{6} = 0$

L'Hôpital's rule holds for **indeterminate forms** $\left[\frac{0}{0}\right]$ or $\left[\frac{\infty}{\infty}\right]$. But what about other indeterminate possibilities?

Try:

$$\lim_{x\to 0+} x^x, \qquad \lim_{x\to 0+} x^{x^x}, \qquad \lim_{x\to 1}\left(\frac{x}{x-1} - \frac{1}{\ln(x)}\right)$$

Indeterminate Forms and L'Hôpital's Rule

- $\lim_{x\to 0+} x^x$: let $y = x^x$, so $\ln(y) = x\ln(x) = \frac{\ln(x)}{1/x}$ $\left[\frac{\infty}{\infty}\right]$
  l'Hôpital: $\lim_{x\to 0+} \frac{\ln(x)}{1/x} = \lim_{x\to 0+} \frac{1/x}{-1/x^2} = \lim_{x\to 0+}(-x) = 0$
  so: $\lim_{x\to 0+} x^x = \lim_{x\to 0+} e^{\ln(y)} = e^{\lim_{x\to 0+}\ln(y)} = e^0 = \boxed{1}$

- $\lim_{x\to 0+} x^{(x^x)}$: since $\lim_{x\to 0+} x^x = 1$, this is NOT indeterminate! $\lim_{x\to 0+} x^{(x^x)} = (\lim_{x\to 0+} x)^{\lim_{x\to 0+} x^x} = 0^1 = \boxed{0}$

- $\lim_{x\to 1}\left(\frac{x}{x-1} - \frac{1}{\ln(x)}\right)$: $= \lim_{x\to 1} \frac{x\ln(x)-x+1}{(x-1)\ln(x)}$ $\left[\frac{0}{0}\right]$
  l'Hôpital: $\lim_{x\to 1} \frac{x\ln(x)-x+1}{(x-1)\ln(x)} = \lim_{x\to 1} \frac{1+\ln(x)-1}{\ln(x)+1-\frac{1}{x}}$ still $\left[\frac{0}{0}\right]$
  l'Hôpital again: $\lim_{x\to 1} \frac{\ln(x)}{\ln(x)+1-\frac{1}{x}} = \lim_{x\to 1} \frac{1/x}{1/x+1/x^2} = \boxed{\frac{1}{2}}$.