Elements of approximation theory

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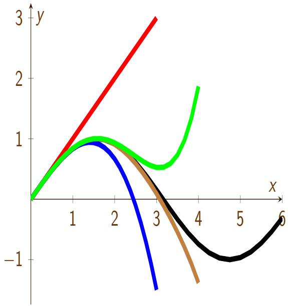
Taylor's formula



Main idea of the Taylor formula is an approximation of given curve by polynomials of different orders. Here one can see the $\sin(x)$ (in black) and the approximation by polynomials of first (red), 3-th (blue), 5-th order (green) and 7-th orders.

Taylor's formula

Let $f(x)$ be a function which has n derivatives at $x = x_0$.

$$f(x) = f(x_0) + f'(\xi)(x - x_0) + k_2(x - x_0)^2 + k_3(x - x_0)^3 + \cdots + k_n(x - x_0)^n + o((x - x_0)^n).$$

$$f''(x) = 2k_2 + 3 \cdot 2 \cdot k_3(x - x_0) + \cdots + o((x - x_0)^{n-2}),$$

$$k_2 = \frac{f''(x_0)}{2},$$

$$f'''(x) = 3 \cdot 2 \cdot 1 \cdot k_3 + \cdots + o((x - x_0)^{n-3}),$$

$$k_3 = \frac{f'''(x_0)}{3 \cdot 2},$$

$$\ddots,$$

$$k_n = \frac{f^{(n)}(x_0)}{n!}.$$

Taylor's formula. Peano form of the remainder.

Theorem.

Let $f(x)$ has derivatives of n-th order at $x = x_0$, then:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(x_0)}{3!}(x - x_0)^3 + \dots + \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n + o((x - x_0)^n).$$

Taylor's formula. Lagrange form of the remainder.

$$f(x) = f(x_0) + \sum_{k=1}^{n-1} \frac{f^{(k)}(x_0)}{k!}(x-x_0)^k + \frac{f^{(n)}(\xi)}{n!}(x-x_0)^n,$$

$$\xi \in (x_0, x).$$

Derivation of the reminder formula

Let's consider

$$\phi(\xi) = f(x) - \sum_{k=0}^{n-1} \frac{f^{(k)(\xi)}}{k!}(x-\xi)^k.$$

Then

$$\phi(x) = 0,\ \phi(x_0) = R_n(x),$$

where $R_n(x)$ is a remainder term.
Define the difference:

$$\phi(x) - \phi(x_0) = \phi'(\xi),\ \xi \in [x, x_0].$$

$$\phi'(\xi) = -\sum_{k=0}^{n-1} \frac{f^{(k+1)}(\xi)}{k!}(x-\xi)^k + \sum_{k=0}^{n-1} \frac{f^{(k)}(\xi)}{(k-1)!}(x-\xi)^{k-1}$$

Derivation of the reminder formula

$$\phi'(\xi) = -\sum_{k=0}^{n-1} \frac{f^{(k+1)}(\xi)}{k!}(x-\xi)^k + \sum_{k=1}^{n-1} \frac{f^{(k)}(\xi)}{(k-1)!}(x-\xi)^{k-1} =$$

$$\sum_{k=1}^{n-1} \left(\frac{f^{(k)}(\xi)}{(k-1)!} - \frac{f^{(k)}(\xi)}{(k-1)!} \right)(x-\xi)^{k-1} - \frac{f^{(n)}(\xi)}{(n-1)!}(x-\xi)^{n-1}.$$

As a result one obtains:

$$\phi(x) - \phi(x_0) = \phi'(\xi)(x - x_0), \;\; \phi'(\xi) = -\frac{f^{(n)}(\xi)}{(n-1)!}(x-\xi)^{n-1}.$$

Derivation of the reminder formula

To obtain the remainder in the Lagrange form use the Cauchy theorem:

$$\frac{\phi(x)-\phi(x_0)}{\psi(x)-\psi(x_0)} = \frac{\phi'(\xi)}{\psi'(\xi)},$$

$$\phi(x)-\phi(x_0) = -\frac{\psi(x)-\psi(x_0)}{\psi'(\xi)}\frac{f^{(n)}(\xi)}{(n-1)!}(x-\xi)^{n-1}.$$

The Lagrange form of the remainder:

$$-\frac{f^{(n)}(\xi)}{n!}(x-x_0)^n = -\frac{\psi(x)-\psi(x_0)}{\psi'(\xi)}\frac{f^{(n)}(\xi)}{(n-1)!}(x-\xi)^{n-1},$$

$$\psi'(\xi) = n(x-\xi)^{n-1},\ \psi(x)=(x-\xi)^n.$$

The remainder in the Lagrange form

$$f(x) = f(x_0) + \sum_{k=1}^{n-1} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + \frac{f^{(n)}(\xi)}{n!}(x - x_0)^n.$$

The Taylor formula. Examples

$$\log(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{6}{(\xi+1)^4}\frac{x^4}{4!}, \ \xi \in (0,x);$$

$$\sqrt{1+x} = 1 + \frac{x}{2} - \frac{x^2}{8} + \frac{x^3}{16} - \frac{15}{16\sqrt{(1+\xi)^7}}x^4, \ \xi \in (0,x).$$

Examples of interpolating polynomials

Suppose we know two points of some function:

$$\{(x_0, y_0), (x_1, y_1)\}, \;\; P_1(x) = \frac{x - x_1}{x_0 - x_1} y_0 + \frac{x - x_0}{x_1 - x_0} y_1 .$$

For three pair of the values we can construct unique polynomial of the second order:

$$\begin{aligned} & \{(x_k, y_k)\}_{k=0}^{2}, \\ P_2(x) \;\; = \;\; & \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} y_0 + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} y_2 + \\ & \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} y_2 . \end{aligned}$$

Lagrange interpolation formula

Suppose we know a set of points of some function:

$$\{(x_k, y_k)\}_{k=0}^{n}.$$

Let $l(x) = \prod_{k=0}^{n}(x - x_k)$. This function is convenient to use for the definition an polynomial which passes thought all of these points:

$$P_n(x) \;=\; \sum_{k=0}^{n} \frac{l(x)}{(x - x_k)l_k} y_k,\;\; l_k = \prod_{j=0, j\neq k}^{n} (x_k - x_j).$$

$P_n(x)$ is called the Lagrange interpolating polynomial.

Interpolation error

Define as $x \neq x_k$:

$$\phi(\xi) = f(\xi) - P_n(\xi) - \lambda l(\xi), \ \ \lambda = \frac{f(x) - P_n(x)}{l(x)}.$$

Hence $\phi(x) = 0$ and $\phi(x_k) = 0, \forall k = 0, \dots, n$. Due to the Rolle's theorem $\phi'(\zeta) = 0$, $\zeta \in (x_j, x_{j+1})$ and the same for $\phi^{(m)}(\zeta)$, $m \leq n+1$:

$$\phi^{(n+1)}(\zeta) = 0. \ \zeta \in (a, b)$$

and

$$\phi^{(n+1)}(\xi) = f^{(n+1)}(\xi) + \lambda (n+1)!, \Rightarrow \lambda = \frac{f^{(n+1)}(\xi)}{(n+1)!}.$$

Then

$$f(x) = P_n(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!} l(x).$$

Examples of interpolating polynomials

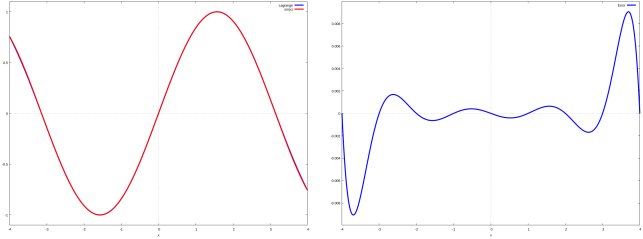


Figure: The Lagrange interpolating polynomial for the $\sin(x)$ at the points $-4, -3, -2, -1, 0, 1, 2, 3, 4.$ and the error of the difference between the interpolating polynomial and $\sin(x)$.

Examples of interpolating polynomials

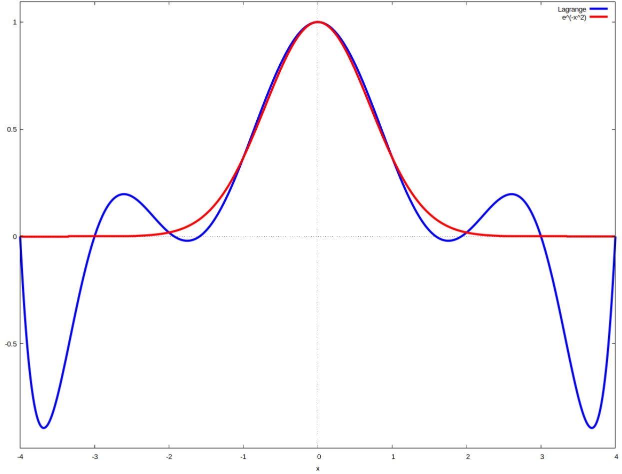


Figure: The Lagrange interpolating polynomial for the e^{-x^2} at the points $-4, -3, -2, -1, 0, 1, 2, 3, 4$.

First definition of the derivative

A derivative is a limit:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{y(x + \Delta x) - y(x)}{\Delta x}.$$

$\forall \varepsilon > 0,\ \exists \delta(\varepsilon) > 0,\ |\Delta x| < \delta$:

$$\left| \frac{y(x + \Delta x) - y(x)}{\Delta x} - \frac{dy}{dx} \right| < \varepsilon.$$

This definition appeals to properties of the curve for a continuous parameter Δx. While a numeric approach assumes a discrete set of allowed values of Δx.

Second definition of the derivative

$$\frac{dy}{dx} = \lim_{n\to\infty} \frac{y(x+\Delta x_n) - y(x)}{\Delta x_n}.$$

$\forall \varepsilon > 0$ and any $\{\Delta x_n\}_{n=1}^{\infty} \to 0,\ \exists N(\varepsilon)$ and:

$$\left| \frac{y(x+\Delta x_n) - y(x)}{\Delta x_n} - \frac{dy}{dx} \right| < \varepsilon.$$

This concept looks close to the numeric approach but basic details are the words any and convergent sequence.

Disclaimer

When we deal with numeric formulas for the derivative then we must understand that we neglect two important ideas of the classical mathematical analysis:

- continuous function;
- continuous of independent variable.

We change the continuous by the a set of values of the floating point numbers.

Disclaimer

Despite of following exaples we will assume that the numbers are a set on a lattice with uniform step Δ..

- Noncommutativity:

```
> > >2.0-0.3+0.3==2.0
true
> > >2.0+0.3-0.3==2.0
false
```

- An errors due to averaging by standard IEEE754

```
> > >z=2.0-0.9
> > >"%.18f" % z
'1.100000000000000089'
```

Approximations of derivatives

Let's consider a Taylor formula for a smooth function $f(x)$ with a residue in the Lagrange form:

$$f(x+\Delta) = f(x) + f'(x)\Delta + O(\Delta^2).$$

It yields:

$$f'(x) = \frac{f(x+\Delta) - f(x)}{\Delta} + O(\Delta).$$

Two-point formula for the derivative

If we consider three terms of the Taylor series:

$$f(x+\Delta) = f(x) + f'(x)\Delta + \frac{f''(x)}{2!}\Delta^2 + O(\Delta^3).$$

Here second derivative is:

$$f''(x) = \frac{1}{\Delta}\left(\frac{f(x+\Delta)-f(x)}{\Delta} - \frac{f(x)-f(x-\Delta)}{\Delta}\right) + O(\Delta) = \frac{f(x+\Delta)-2f(x)+f(x-\Delta)}{\Delta^2} + O(\Delta).$$

In this case:

$$f(x+\Delta) = f(x)+f'(x)\Delta+\frac{f(x+\Delta)-2f(x)+f(x-\Delta)}{2!}+O(\Delta^3)$$

and

$$f'(x) = \frac{f(x+\Delta)-f(x-\Delta)}{2\Delta} + O(\Delta^2).$$

Two two-point formulas for the derivative

$$
\begin{aligned}
f'(x) &= \frac{f(x+\Delta)-f(x)}{\Delta} + O(\Delta), \\
f'(x) &= \frac{f(x+\Delta)-f(x-\Delta)}{2\Delta} + O(\Delta^2).
\end{aligned}
$$

Four-point formulas for the derivative

The four terms of the Taylor series:

$$f(x+\Delta) \sim f(x) + f'(x)\Delta + \frac{f''(x)}{2!}\Delta^2 + \frac{f'''(x)}{3!}\Delta^3.$$

Here

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

Then:

$$f'(x) = \frac{1}{12\Delta}(f(x+2\Delta) - 8f(x+\Delta) + 8f(x-\Delta) - f(x-2\Delta)) + O(\Delta^4).$$

Formulas for first derivative

$$f'(x) = \frac{f(x+\Delta) - f(x)}{\Delta} + O(\Delta),$$

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

$$f'(x) = \frac{1}{12\Delta}(f(x+2\Delta) - 8f(x+\Delta) + +8f(x-\Delta) - f(x-2\Delta)) + O(\Delta^4).$$

Examples

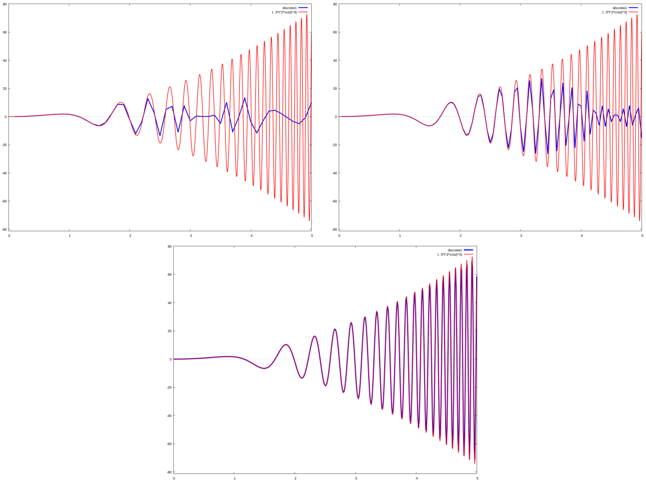


Figure: The numeric derivative of $\sin(x^3)$ on the interval $x \in [0, 5]$ with steps 0.1, 0.05, 0.01.

General formula for the numeric integration

$$\int_a^b f(x)dx = \sum_{k=0}^{N} c_k f(x_k) + R.$$

Here

- x_k is a knot of the lattice;
- N is the number of the number of the knots in the interval $[a, b]$;
- c_k is a weight coefficient;
- R is the residue term, which is difference between the approximation sum and the value of the integral.

The simplest case

Let's consider an uniform lattice of N knots on the interval and $x_{k+1} - x_k = (b-a)/N = \Delta$.

$$f(x) = f(x_k) + O(\Delta), \quad x \in [x_k, x_{k+1}),$$

so

$$\int_a^b f(x)dx = \sum_{k=0}^{N} f(x_k)\Delta + O(\Delta).$$

Trapezoidal approximation

$$f(x) = f(x_k) + \frac{f(x_{k+1} - f(x_k)}{\Delta}x + O(\Delta^2), \quad x \in [x_k, x_{k+1}],$$

Then integral over the interval $x \in [x_k, x_{k+1}]$:

$$\int_{x_k}^{x_{k+1}} \left(f(x_k) + \frac{f(x_{k+1}) - f(x_k)}{\Delta}x \right) dx =$$

$$f(x_k)\Delta + \frac{1}{2\Delta}f(x_{k+1})\Delta^2 - \frac{1}{2\Delta}f(x_k)\Delta^2 =$$

$$\frac{1}{2}(f(x_{k+1}) + f(x_k))\Delta.$$

Trapezoidal approximation

$$\int_a^b f(x)dx = \sum_{k=0}^{N-1} \int_{x_k}^{x_{k+1}} \left(f(x_k) + \frac{f(x_k) - f(x_{k+1})}{\Delta} x \right) dx + O(\Delta^2) = \sum_{k=0}^{N-1} \frac{1}{2}(f(x_{k+1}) + f(x_k))\Delta + O(\Delta^2)$$

As a result:

$$\int_a^b f(x)dx = \frac{1}{2} f(x_0)\Delta + \sum_{k=1}^{N-1} f(x_k)\Delta + \frac{1}{2} f(x_N)\Delta + O(\Delta^2).$$

Formulas for integration over finite interval

$$\int_a^b f(x)dx = \sum_{k=0}^{N} f(x_k)\Delta + O(\Delta).$$

$$\int_a^b f(x)dx = \frac{1}{2}f(x_0)\Delta + \sum_{k=1}^{N-1} f(x_k)\Delta + \frac{1}{2}f(x_N)\Delta + O(\Delta^2).$$

A high order approximation one can obtain if one chose a formula for high level of approximation of the curve on the elementary interval.

An example

$$\int_0^{2\pi} \sin(x^3)dx \sim 0.4548524546$$

The same integral calculated by the trapezoid method with step 0.0001 :

$$0.45483$$

Summary