BSc Mathematics for Computer Scientists 2: X. Root Finding, Approximation of Real Functions by Polynomials, Power Series

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Root Finding: The Basic Problem

Problem

Given: $f : [a, b] \to \mathbb{R}$ a continuous function, differentiable on the interval $]a, b[$.
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- We present two methods.

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Stopping rule: If the length of I_n is smaller than ϵ, we stop. Otherwise, we return to the Update rule.

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Assume that initially the current interval has unit length, i.e., its length is 1.
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Based on the theorem, any point in the current interval gives an approximation of the guaranteed root such that the error is at most $\frac{1}{2^k}$. In particular, after k updates the approximation is "accurate to k digits in the binary number system".

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• **Idea for the update:** After approximating the root by x_n, we proceed using the tangent.

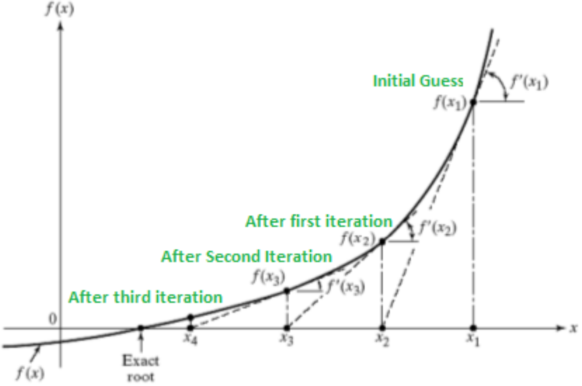
At the point x_n, we write the equation of the tangent:

$$y = f(x_n) + f'(x_n)(x - x_n)$$

We find the root of the tangent equation (a linear equation)$\rightarrow x_{n+1}$. That is, we find the intersection of the tangent with the x-axis ($y = 0$):

$$0 = f(x_n) + f'(x_n)(x_{n+1} - x_n) \quad \Rightarrow \quad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Root Finding: Newton's Method: Illustration



Forrás:
https://predictivehacks.com/newton-raphson-method-in-python/

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Warning: It does not work if $f'(x_n) = 0$, for example if x_n is a local minimum/maximum. The precise formulation of the algorithm is more technical. Our goal is not completeness.

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• We note that if x_n enters a "basin of attraction" of a root r, then the method converges to the root very quickly.

• The success of the algorithm depends on how quickly we get a sufficiently good approximation of the root.

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Root Finding: Newton's Method: Application

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- $x_0 = 1.5$ is a good "guess" for the initial value.
- $$x_{n+1} = x_n - \frac{x_n^2 - 2}{2x_n} = \frac{x_n + \frac{2}{x_n}}{2}$$

Based on this, define a sequence:

$x_1 = \frac{1.5 + \frac{2}{1.5}}{2} = \frac{17}{12} = 1.416666667$, $x_2 = \frac{577}{408} = 1.414215686$, $x_3 = \frac{665857}{470832} = 1.414213562$.

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- $|x_2 - x_3|$ is already very small. $\sqrt{2} \approx \frac{665857}{470832}$. In fact,

$$\left(\frac{665857}{470832}\right)^2 = \frac{443365544449}{221682772224} = 2 + \frac{1}{221682772224}.$$

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- This method was already known to the Babylonians, even though derivatives were not yet known at that time.

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• Light chooses a path between points P and Q located on two sides of a line. On one side of the line it travels with speed v_1, on the other side with speed v_2. What path does it follow?

Optimization: Observations

- The light ray must reach the line at a point O. The path consists of segments PO and OQ, each lying in a homogeneous medium. Here minimal time is equivalent to minimal distance. The path of minimal length is the straight segment PO and the straight segment OQ.

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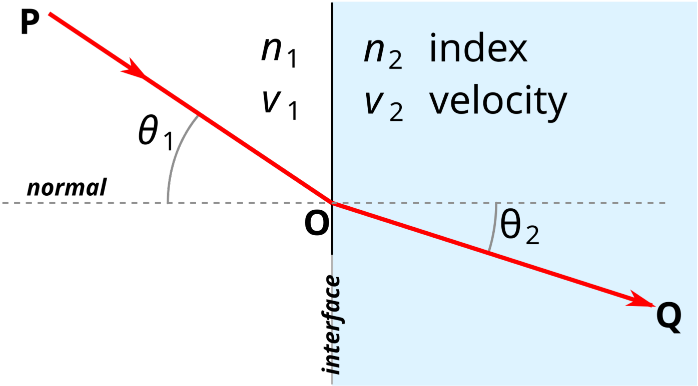

Optimization: Formalization

- Let the equation of the line be $x = 0$. Let $P(-a, 0)$ and $Q(b, -c)$, where $a, b, c > 0$.

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- The total time:

$$T(x) = \frac{\sqrt{x^2 + a^2}}{v_1} + \frac{\sqrt{(c - x)^2 + b^2}}{v_2}.$$

By Fermat's principle, we seek the minimum of $T(x)$.

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$$\frac{\sin\theta_1}{v_1} = \frac{\sin\theta_2}{v_2},$$

where θ_1 is the angle of incidence and θ_2 is the angle of refraction.

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Theorem [Snell–Descartes Law]

For the path of the refracted light ray:

$$n_1 \sin\theta_1 = n_2 \sin\theta_2,$$

where $n = c/v$ is the refractive index.

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$$\mathbb{R}[x] = \{0\} \cup \{p(x) : p(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_d x^d, \text{ where } a_0, a_1, a_2, \ldots, a_d \in \mathbb{R}, a_d \neq 0\}$$

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- Polynomials are continuous and infinitely differentiable. The derivative can be computed easily and efficiently.

- We approximate arbitrary (even complicated) functions $f : [a, b] \to \mathbb{R}$ by polynomials.

- When do we consider an approximation good? Which of two approximations is better?

Polynomials: Interpolation: Basic question

Given a function $f : [a, b] \to \mathbb{R}$.

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Find a polynomial $p \in \mathbb{R}[x]$ such that

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That is, fit a "low-degree" polynomial to the data coming from f.

Theorem

Given places $t_1 < t_2 < \ldots < t_n$ and values φ_1, φ_2, ..., φ_n. Then there exists exactly one polynomial p of degree at most $n-1$ such that

$$\varphi_1 = f(t_1), \quad \varphi_2 = f(t_2), \quad \ldots, \quad \varphi_n = f(t_n).$$

Polynomials: Interpolation: Lagrange

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- The theorem contains two statements: existence and uniqueness.
- We outline two approaches to prove the theorem.

Polynomials: Interpolation: Lagrange: First proof

Given $t_1 < t_2 < \ldots < t_n$ and φ_1, φ_2, …, φ_n real numbers.

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We seek a polynomial $p(x)$ / coefficients $a_0, a_1, \ldots, a_{n-1} \in \mathbb{R}$ such that

$$\begin{array}{ccc} a_0 + a_1 t_1 + a_2 t_1^2 + & \ldots & + a_{n-1} t_1^{n-1} = \varphi_1 \\ a_0 + a_1 t_2 + a_2 t_2^2 + & \ldots & + a_{n-1} t_2^{n-1} = \varphi_2 \\ & \vdots & \\ a_0 + a_1 t_n + a_2 t_n^2 + & \ldots & + a_{n-1} t_n^{n-1} = \varphi_n. \end{array} \tag{1}$$

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• We have n linear conditions for the unknowns $a_0, a_1, a_2, \ldots, a_{n-1}$ (n unknowns).

Given $t_1 < t_2 < \ldots < t_n$ and $\varphi_1, \varphi_2, \ldots, \varphi_n$ real numbers.

We seek a polynomial $p(x)$ / coefficients $a_0, a_1, \ldots, a_{n-1} \in \mathbb{R}$ such that

$$\begin{aligned} a_0 + a_1 t_1 + a_2 t_1^2 + \quad &\ldots \quad + a_{n-1} t_1^{n-1} = \varphi_1 \\ a_0 + a_1 t_2 + a_2 t_2^2 + \quad &\ldots \quad + a_{n-1} t_2^{n-1} = \varphi_2 \\ &\vdots \\ a_0 + a_1 t_n + a_2 t_n^2 + \quad &\ldots \quad + a_{n-1} t_n^{n-1} = \varphi_n. \end{aligned} \tag{1}$$

- We have n linear conditions for the unknowns $a_0, a_1, a_2, \ldots, a_{n-1}$ (n unknowns).
- The coefficient matrix of the system is

$$M_L = \begin{pmatrix} 1 & t_1 & t_1^2 & \ldots & t_1^{n-1} \\ 1 & t_2 & t_2^2 & \ldots & t_2^{n-1} \\ \vdots & & & & \vdots \\ 1 & t_n & t_n^2 & \ldots & t_n^{n-1} \end{pmatrix}.$$

Polynomials: Interpolation: Lagrange: First proof

Theorem

(i) The system of equations (1) has a unique solution.

(ii)
$$\det M_L = \prod_{1 \le i < j \le n} (t_i - t_j) \neq 0.$$

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$$\det M_L = \prod_{1\le i<j\le n} (t_i - t_j) \neq 0.$$

- The remaining part of the proof follows from linear algebra.

Polynomials: Interpolation: Lagrange: Second proof

Theorem

Given places $t_1 < t_2 < \ldots < t_n$. Then there exist polynomials $p_i \in \mathbb{R}[x]$ ($i = 1, 2, \ldots, n$) such that

$$p_i(t_1) = p_i(t_2) = \ldots = p_i(t_{i-1}) = p_i(t_{i+1}) = p_i(t_{i+2}) = \ldots = p_i(t_n) = 0,$$

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Given places $t_1 < t_2 < \ldots < t_n$. Then there exists a polynomial $p \in \mathbb{R}[x]$ such that

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- Uniqueness can be proven independently.

Break

Weierstrass approximation: The basic question

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If f is not continuous, then such a polynomial certainly does not exist.

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If f is not continuous, then such a polynomial certainly does not exist.

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From now on, assume that the function f is continuous.

Weierstrass approximation: The main theorem

Theorem: Weierstrass approximation theorem

Let $f : [a, b] \to \mathbb{R}$ be any continuous function. Given an arbitrary $\varepsilon > 0$. Then there exists a polynomial $p_\varepsilon(x) \in \mathbb{R}[x]$ such that

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- Without loss of generality, we may assume that $[a, b] = [0, 1]$.
- Let (the n-th degree Bernstein polynomial of f on $[0, 1]$):

$$B_{f,n}(x) = \sum_{k=0}^{n} f\left(\frac{k}{n}\right)\binom{n}{k}x^k(1-x)^{n-k}.$$

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- We verify that for any $\varepsilon > 0$, a sufficiently large degree $B_{f,n}(x)$ is appropriate. This is technical, so we omit the verification.

Weierstrass approximation: Example

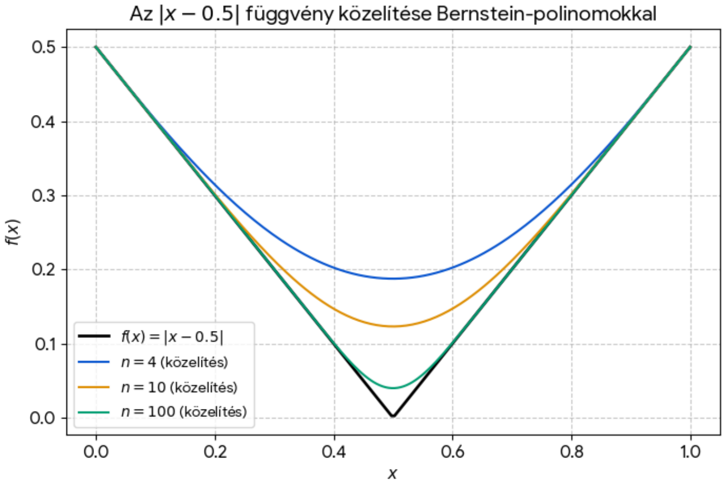

Figure: Three approximations of the function $f(x) = |x - 0.5|$ on the interval $[0, 1]$.

Weierstrass approximation: Example: Explanation

- 4th-degree approximating polynomial (blue graph).

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Bernstein formula:

$$\begin{aligned} P_4(x) &= \sum_{k=0}^{4} \left|\frac{k}{4} - 0.5\right| \binom{4}{k} x^k (1-x)^{4-k} \\ &= 0.5(1-x)^4 + 0.25 \cdot 4x(1-x)^3 + 0.25 \cdot 4x^3(1-x) + 0.5x^4. \end{aligned}$$

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The formula ($\epsilon \approx 0.079$):

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Break

Taylor Polynomials: Introduction

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Reminder

Let $f : (a, b) \to \mathbb{R}$ be a differentiable function. Let $x_0 \in \mathrm{dom}(f)$. The linear function ℓ that best approximates f ($\ell(x_0) = f(x_0)$, $\ell'(x_0) = f'(x_0)$):

$$\ell(x) = f(x_0) + f'(x_0)(x - x_0) \approx f(x).$$

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- Let us look for a quadratic polynomial $q(x) = a(x - x_0)^2 + b(x - x_0) + c$ such that $q(x_0) = f(x_0)$, $q'(x_0) = f'(x_0)$ and $q''(x_0) = f''(x_0)$

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- Writing out the conditions:

$$\begin{aligned} q(x_0) &= c = f(x_0), \\ q'(x_0) &= b = f'(x_0), \\ q''(x_0) &= 2a = f''(x_0). \end{aligned}$$

Taylor Polynomials: The first steps

Observation

Let $f : (a, b) \to \mathbb{R}$ be a twice differentiable function. Let $x_0 \in \mathrm{dom}(f)$.
Then there exists exactly one polynomial of degree at most 2 such that $q(x_0) = f(x_0)$, $q'(x_0) = f'(x_0)$ and $q''(x_0) = f''(x_0)$. This polynomial is:

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- Notice the similarity with the linear algebraic solution of the Lagrange interpolation theorem.
- The generalization is straightforward.

Taylor Polynomials: Definition

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Let $f : (a, b) \to \mathbb{R}$ be an n times differentiable function. Let $x_0 \in \mathrm{dom}(f)$. Then there exists exactly one polynomial of degree at most n such that $p_{f,n,x_0}(x_0) = f(x_0)$, $p'_{f,n,x_0}(x_0) = f'(x_0)$, $\ldots$, $p^{(n)}_{f,n,x_0}(x_0) = f^{(n)}(x_0)$. This polynomial is:

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Definition

The polynomial in the previous theorem is called the n-th order Taylor polynomial of f around x_0. Its notation is T_{f,n,x_0}. If f and x_0 are clear from the context, we simply write $T_n(x)$.

Taylor Polynomials: Remainder

Definition: Remainder (error term) of the Taylor polynomial

$$R_{f,n,x_0}(x) = f(x) - T_{f,n,x_0}(x),$$

that is $f(x) = T_{f,n,x_0}(x) + R_{f,n,x_0}(x)$.

Taylor Polynomials: Remainder

Definition: Remainder (error term) of the Taylor polynomial

$$R_{f,n,x_0}(x) = f(x) - T_{f,n,x_0}(x),$$

that is $f(x) = T_{f,n,x_0}(x) + R_{f,n,x_0}(x)$.

- $R_{f,n,x_0}(x)$ measures the deviation between the original function $f(x)$ and the n-th order Taylor polynomial $T_n(x)$.

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- If f and x_0 are clear from the context, we simply write $R_n(x)$.

Taylor Polynomials: Remainder Estimates

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Theorem [Lagrange]

$$R_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}, \quad \text{where } \xi \text{ lies between } x_0 \text{ and } x$$

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Theorem [Peano]

$$R_n(x) = o((x-x_0)^n).$$

Taylor Polynomials: Formal Power Series

Definition

$$a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + \ldots + a_n(x - x_0)^n + \ldots$$

is called a (real) formal power series. Its set is denoted by $\mathbb{R}[[x]]$.

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Definition

Let

$f = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + \ldots + a_n(x - x_0)^n + \ldots \in \mathbb{R}[[x]]$.

The radius of convergence of f is R, where $R = \sup\{\rho\} \in \widehat{\mathbb{R}}$. Here $\{\rho\}$ is the set of non-negative ρ such that for $x_1 \in (x_0 - \rho, x_0 + \rho)$ the

$$a_0 + a_1(x_1 - x_0) + a_2(x_1 - x_0)^2 + \ldots + a_n(x_1 - x_0)^n + \ldots$$

infinite numerical sum is defined.

Taylor Polynomials: Formal Power Series: Radius of Convergence

The radius of convergence R of a formal power series $f \in \mathbb{R}[[x]]$ lies in $[0, \infty]$. We give another, more computable description.

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Theorem

$$R = \frac{1}{\limsup_{n\to\infty} |c_n|^{1/n}}.$$

Here $\limsup_{n\to\infty} s_n$ denotes the supremum of the accumulation points (of the sequence s_n in $\widehat{\mathbb{R}}$). It may be $0^+ = 0$ (the $+$ indicates non-negative sequences) or ∞. Recall that $\frac{1}{\infty}$ has been defined. It is natural to adopt the convention $\frac{1}{0^+} = \infty$.

Taylor Polynomials: Formal Power Series: Radius of Convergence: Background

The theorem on the radius of convergence follows easily from results on numerical series. Let

$$\sum_{n=0}^{\infty} s_n$$

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Theorem [Ratio Test]

Assume that $\lim_{n\to\infty} \frac{|s_{n+1}|}{|s_n|} = q$. Then

(i) If $|q| < 1$, then the series is absolutely convergent,

(ii) If $|q| > 1$, then the series is divergent.

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Taylor Polynomials: Formal Power Series: Radius of Convergence: Background (continued)

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Definition

The Taylor series of f (around x_0) is

$$f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2}(x-x_0)^2 + \frac{f'''(x_0)}{3!}(x-x_0)^3 + \ldots + \frac{f^{(n)}(x_0)}{n!}(x-x_0)^n + \ldots \in \mathbb{R}[[x]].$$

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- On the interval $(x_0 - R, x_0 + R)$ the Taylor series defines a function. What is the relation between this function and f?

Taylor Polynomials: Taylor Series: Example

Example

$$f(x) = \begin{cases} e^{-1/x^2}, & \text{if } x \neq 0, \\ 0, & \text{if } x = 0. \end{cases}$$

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For this function:

- $\mathrm{dom}(f) = \mathbb{R}$,
- it is infinitely differentiable on $\mathbb{R} \setminus \{0\}$,
- it is ALSO infinitely differentiable at 0,
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Theorem

The Taylor series of f is

$$0 + 0 \cdot x + 0 \cdot x^2 + 0 \cdot x^3 + 0 \cdot x^4 + \ldots \equiv 0.$$

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Theorem

The Taylor series of f is

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This Taylor series is absolutely convergent everywhere, but it coincides with $f(x)$ only at $x = 0$.

Definition

Let f be a real-valued function defined on an open interval. We say that f is (real) analytic if around every $x_0 \in \mathrm{dom}(f)$ it can be represented as a function defined by a power series.

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Theorem

If an analytic function f can be represented around $x_0 \in \mathrm{dom}(f)$ by a power series, then this series must be the Taylor series of f at x_0.

Analytic Functions: Examples

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Example

$\frac{1}{1-x}$ is analytic on $]-1,1[$ and here

$$\frac{1}{1-x}=\sum_{n=0}^{\infty}x^n=1+x+x^2+x^3+\dots$$

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Example

e^x is analytic on $\mathbb{R}$ and here

$$e^x=\sum_{n=0}^{\infty}\frac{x^n}{n!}=1+x+\frac{x^2}{2!}+\frac{x^3}{3!}+\dots$$

Analytic functions: Examples

Example

$\sin x$ is analytic on $\mathbb{R}$ and here

$$\sin(x) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!} = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \dots$$

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$\cos x$ is analytic on $\mathbb{R}$ and here

$$\cos(x) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n}}{(2n)!} = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \dots$$

Example

$\ln x$ is analytic on $]-1,1[$ and here

$$\ln(1+x)=\sum_{n=1}^{\infty}(-1)^{n+1}\frac{x^n}{n}=x-\frac{x^2}{2}+\frac{x^3}{3}-\dots$$

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Example

$\frac{x}{e^x-1}$ is analytic on $\mathbb{R}$ and here

$$\frac{x}{e^x-1}=\sum_{n=0}^{\infty}B_n\frac{x^n}{n!}=B_0+B_1x+\frac{B_2}{2!}x^2+\frac{B_3}{3!}x^3+\dots,$$

where $\{B_n\}$ is the sequence of Bernoulli numbers.

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$\tan x$ is analytic on $\left]-\frac{\pi}{2}, \frac{\pi}{2}\right[$ and here

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Example

$(1+x)^\alpha$ $(\alpha \in \mathbb{R})$ is analytic on $]-1,1[$ and here

$$(1+x)^\alpha = \sum_{n=0}^{\infty} \binom{\alpha}{n} x^n = 1 + \alpha x + \frac{\alpha(\alpha-1)}{2!} x^2 + \dots$$

Analytic functions: "They are nice"

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Theorem

Let $f(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + \dots$ and $g(x) = b_0 + b_1x + b_2x^2 + b_3x^3 + \dots$ be two analytic functions ($0 \in \mathrm{dom}(f) = \mathrm{dom}(g)$). Then

(i) fg is analytic, and

$$fg(x) = a_0b_0 + (a_0b_1 + a_1b_0)x + (a_0b_2 + a_1b_1 + a_2b_0)x^2 + \dots$$

(ii) f' is analytic, and

$$f'(x) = a_1 + 2a_2x + 3a_2x^2 + 4a_3x^3 + \dots$$

That is, analytic functions can be handled formally and conveniently. In particular, they can be differentiated term by term.

Analytic functions: Turning them into pennies

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$$\sqrt{1 + 0.001} \approx 1 + \frac{1}{2}0.001,$$

$$\ln(1 + 0.1) \approx 0.1 - \frac{1}{2}0.1.$$

Thank you for your attention!