## Approximation Theory and Proof Assistants: Certified Computations

Nicolas Brisebarre and Damien Pous

Master 2 Informatique Fondamentale École Normale Supérieure de Lyon, 2024-2025 Let w be a weight function over (a, b), and let  $f \in C([a, b])$ . We briefly study methods which approximate the integral

$$\int_{a}^{b} f(x)w(x)\mathrm{d}x$$

with a sum of the form

$$\sum_{k=0}^n w_k f(x_k), \qquad w_k \in \mathbb{R}, \quad x_k \in [a,b] \text{ pairwise distinct}$$

## Section 2.2. A little bit of quadrature: Gauss methods

First of all, if 
$$\ell_k(x) = \prod_{\substack{j=0,\ j \neq k}}^n \frac{x-x_j}{x_k-x_j}$$
, observe that if

$$p(x) = \sum_{k=0}^{n} f(x_k)\ell_k(x) \in \mathbb{R}_n[x]$$

interpolates f at the points  $x_0, \ldots, x_n$ , then our approximation for the integral is equal to  $\int_a^b p(x)w(x)dx = \sum_{k=0}^n w_k f(x_k)$  with

$$w_k = \int_a^b \ell_k(x) w(x) \mathrm{d}x$$
 for  $k = 0, \dots, n$ .

There exists a unique choice of the points  $x_k$  and the weights  $w_k$  such that, whenever  $f \in \mathbb{R}_{2n+1}[x]$ ,

$$\int_{a}^{b} f(x)w(x)\mathrm{d}x = \sum_{k=0}^{n} w_{k}f(x_{k}).$$

These points  $x_k$  belong to (a, b) and are the roots of the (n + 1)-th orthogonal polynomial associated to w.

# Section 2.2. A little bit of quadrature: Clenshaw-Curtis quadrature

#### Remark

The Chebyshev polynomials of the first kind satisfy

$$\int_{-1}^{1} T_k(x) \mathrm{d}x = \begin{cases} \frac{2}{1-k^2}, & k \in 2\mathbb{N}, \\ 0, & k \notin 2\mathbb{N}. \end{cases}$$

If  $p = \sum_{k=0}^{n} c_k T_k$ , we deduce that the integral with weight w = 1 is given by

$$\int_{-1}^{1} p(x) \mathrm{d}x = \sum_{\substack{0 \leq k \leq n \\ k \in 2\mathbb{N}}} \frac{2c_k}{1-k^2}.$$

## Section 2.3. Lebesgue constants

For simplicity, we assume [a, b] = [-1, 1].

#### Definition 9

We say that a linear mapping  $L : C([-1,1]) \to \mathbb{R}_n[x]$  is a projection onto  $\mathbb{R}_n[x]$  if Lp = p for all  $p \in \mathbb{R}_n[x]$ . The operator norm

$$\Lambda = \sup_{f \in \mathcal{C}([-1,1])} \frac{\|Lf\|_{\infty}}{\|f\|_{\infty}}$$

is called the Lebesgue constant for the projection.

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#### Proposition

Let  $\Lambda$  be the Lebesgue constant for the linear projection L of C([-1,1])onto  $\mathbb{R}_n[x]$ . Let  $f \in C([-1,1])$  and let p = Lf. Let  $p^*$  denote the minimax approximation to f. Then, we have

$$||f - p||_{\infty} \leq (1 + \Lambda) ||f - p^*||_{\infty}.$$

## 2.3.1. Lebesgue constants for polynomial interpolation

Let  $x_0, \ldots, x_n$  be pairwise distinct points in [-1, 1]. Consider the Lagrange interpolation operator

$$L_n: \mathcal{C}([-1,1]) \to \mathbb{R}_n[x], \qquad L_n f(x) = \sum_{k=0}^n f(x_k)\ell_k(x).$$

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#### Theorem 10

The Lebesgue constant of degree-n Lagrange interpolation at  $x_0, \ldots, x_n$  is equal to

$$\max_{x \in [-1,1]} \sum_{k=0}^{n} |\ell_k(x)|.$$

## 2.3.1. Lebesgue constants for polynomial interpolation

#### Theorem 11

The Lebesgue constant  $\Lambda_n$  satisfies

$$\frac{2}{\pi} \left( \log(n+1) + \gamma + \log \frac{4}{\pi} \right) \leqslant \Lambda_n, \text{ where } \frac{2}{\pi} \left( \gamma + \log \frac{4}{\pi} \right) = 0.52125\dots$$

#### Additionally,

• for Chebyshev nodes (of the first and the second kinds), we have the bound

$$\Lambda_n \leqslant \frac{2}{\pi} \log(n+1) + 1 \text{ and } \Lambda_n \sim \frac{2}{\pi} \log n \text{ as } n \to +\infty;$$

• for equispaced points,

$$\Lambda_n > \frac{2^{n-2}}{n^2} \text{ and } \Lambda_n \sim \frac{2^{n+1}}{en\log n} \text{ as } n \to +\infty$$

#### Remark

We deduce from this theorem that Chebyshev interpolants (i.e. interpolation polynomials at Chebyshev nodes) are "near-best" approximations:

- Λ<sub>15</sub> = 2.76...: one loses at most 2 bits if one uses a Chebyshev interpolant instead of the minimax polynomial;
- $\Lambda_{30} = 3.18...$ : one loses at most 2 bits if one uses a Chebyshev interpolant instead of the minimax polynomial;
- Λ<sub>100</sub> = 3.93...: one loses at most 2 bits if one uses a Chebyshev interpolant instead of the minimax polynomial;
- $\Lambda_{100000} = 8.32...$ : one loses at most 4 bits if one uses a Chebyshev interpolant instead of the minimax polynomial.

When the  $L_2$  space under consideration is  $L_2\left([-1,1],\frac{1}{\sqrt{1-x^2}}\right)$ , the best polynomial approximation  $p_{2,n}$  is called the truncated Chebyshev series of order n.

#### Theorem 12

The Lebesgue constant for the  $L_2\left([-1,1],\frac{1}{\sqrt{1-x^2}}\right)$  projection onto  $\mathbb{R}_n[x]$  is

$$\Lambda_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left| \frac{\sin((n+1/2)t)}{\sin(t/2)} \right| \mathrm{d}t.$$

We have

$$\Lambda_n \leqslant \frac{4}{\pi^2} \log(n+1) + 3 \text{ and } \Lambda_n \sim \frac{4}{\pi^2} \log n \text{ as } n \to +\infty.$$

#### Remark

We deduce from this theorem that truncated Chebyshev series are "near-best" approximations:

- Λ<sub>15</sub> = 4.12...: one loses at most 3 bits if one uses the truncated Chebyshev series instead of the minimax polynomial;
- Λ<sub>30</sub> = 4.39...: one loses at most 3 bits if one uses the truncated Chebyshev series instead of the minimax polynomial;
- $\Lambda_{100} = 4.87...$ : one loses at most 3 bits if one uses the truncated Chebyshev series instead of the minimax polynomial;
- Λ<sub>100000</sub> = 7.66...: one loses at most 3 bits if one uses the truncated Chebyshev series instead of the minimax polynomial.

# 2.3.3. Corollary: A first statement on the convergence of Chebyshev interpolants and truncated Chebyshev series

Let  $f \in \mathcal{C}([a,b]).$  The modulus of continuity of f is the function  $\omega$  defined as

for all 
$$\delta > 0$$
,  $\omega(\delta) = \sup_{\substack{|x-y| < \delta, \\ x, y \in [a, b]}} |f(x) - f(y)|$ .

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#### Proposition

If f is a continuous function over [0,1],  $\omega$  its modulus of continuity, then we have

$$||f - B_n(f, \cdot)||_{\infty} = \frac{9}{4}\omega\left(n^{-\frac{1}{2}}\right).$$

# 2.3.3. Corollary: A first statement on the convergence of Chebyshev interpolants and truncated Chebyshev series

#### Theorem 13

If f is Lipschitz continuous over [a, b], then

- the sequence of interpolation polynomials at the Chebyshev nodes uniformly converges to *f*.
- **2** The truncated Chebyshev series of f uniformly converges to f.

## Section 2.4.2. Convergence

#### Remark

The Chebyshev expansion of f is the Fourier expansion of  $f(\cos t)$ , so that many results on the convergence of Chebyshev expansions can be deduced from corresponding results in the well-developed theory of Fourier series.

Let f be continuous on [-1,1]. Denote by  $(a_k)$  its sequence of Chebyshev coefficients, by  $(f_n)$  its sequence of truncated Chebyshev expansions and by  $(p_n)_{n\in\mathbb{N}}$  the sequence of interpolation polynomials of f at the Chebyshev nodes. Then

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- **1** The coefficients  $a_k$  tend to 0 when  $k \to \infty$ .
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- **2** If f is Lipschitz continuous on [-1,1], then  $(f_n)$  converges absolutely and uniformly to f and  $(p_n)$  converges uniformly to f.
- 3 If f is  $C^m$  and  $f^{(m)}$  is Lipschitz continuous, then  $a_k = O(1/k^{m+1})$ ,  $\|f f_n\|_{\infty} = O(n^{-m})$  and  $\|f p_n\|_{\infty} = O(n^{-m})$ .

Let 
$$\rho > 1$$
, let  
 $\mathcal{E}_{\rho} := \left\{ \frac{\rho e^{i\theta} + \rho^{-1} e^{-i\theta}}{2}, \theta \in [0, 2\pi] \right\} = \left\{ z \in \mathbb{C} : |z + \sqrt{z^2 - 1}| \leqslant \rho \right\}.$ 



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• If f is analytic inside the ellipse 
$$\mathcal{E}_{\rho} := \left\{ \frac{\rho e^{i\theta} + \rho^{-1} e^{-i\theta}}{2}, \theta \in [0, 2\pi] \right\} = \left\{ z \in \mathbb{C} : |z + \sqrt{z^2 - 1}| \leq \rho \right\}$$
  
with  $\rho > 1$ , then  $a_k = O(\rho^{-k})$ ,  $||f - f_n||_{\infty} = O(\rho^{-n})$  and  $||f - p_n||_{\infty} = O(\rho^{-n})$ .

## Section 2.4.2. Convergence

#### Theorem 16

Let f be continuous on [-1,1]. Denote by  $(f_n)$  its sequence of truncated Chebyshev expansions and by  $(p_n)_{n\in\mathbb{N}}$  the sequence of interpolation polynomials of f at the Chebyshev nodes. Then

O Let P<sup>\*</sup><sub>n</sub> denote the minimax polynomial of degree at most n of f. If f ∈ C<sup>n+1</sup>([-1,1]), there exists ξ<sub>1</sub>,ξ<sub>2</sub>,ξ<sub>3</sub> ∈ (-1,1) such that

$$\|f - P_n^*\|_{\infty} = \frac{|f^{(n+1)}(\xi_1)|}{2^n(n+1)!};$$
  
$$\|f - f_n\|_{\infty} = \frac{|f^{(n+1)}(\xi_2)|}{2^n(n+1)!};$$
  
$$\|f - p_n\|_{\infty} = \frac{|f^{(n+1)}(\xi_3)|}{2^n(n+1)!}.$$

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## Chapter 3. Interval Arithmetic, Interval Analysis

# Floating Point (FP) Arithmetic

Given

$$\left\{ \begin{array}{ll} \text{a radix} & \beta \geqslant 2, \\ \text{a precision} & p \geqslant 1, \\ \text{a set of exponents} & E_{\min}, \cdots, E_{\max}. \end{array} \right.$$

A finite FP number  $\boldsymbol{x}$  is represented by 2 integers:

- integer mantissa : M,  $\beta^{p-1} \leq |M| \leq \beta^p 1$ ;
- exponent E,  $E_{\min} \leq E \leq E_{\max}$

such that

$$x = \frac{M}{\beta^{p-1}} \times \beta^E.$$

We assume binary FP arithmetic (that is to say  $\beta = 2$ .) We denote  $\mathcal{F}_p$  the corresponding set of FP numbers. Multiple-precision FP arithmetic: we let p and E vary.



See http://en.wikipedia.org/wiki/IEEE\_floating\_point

	precision	minimal exponent	maximal exponent
single (binary 32)	24	-126	127
double (binary 64)	53	-1022	1023
extended double	64	-16382	16383
quadruple (binary 128)	113	-16382	16383

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IEEE standard defines 4 different rounding modes:

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 $\circ_d(x) = \max\{y \in \mathcal{F}_p : y \leqslant x\};\$ 

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- rounding towards 0:  $\circ_z(x) := \circ_u(x)$  if x < 0, and to  $\circ_d(x)$  otherwise;
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- rounding to the nearest even:  $\circ_n(x)$  is the element of  $\mathcal{F}_p$  that is closest to x. If x is exactly halfway between two consecutive elements of  $\mathcal{F}_p$ ,  $\circ_n(x)$  is the one for which the integral significand j is an even number.

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The first three rounding modes are called directed rounding modes.

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Assume for instance that we know that  $5 \le a \le 6$  and  $10 \le b \le 11$ : then of course  $50 \le ab \le 66$ . We will define a product of real intervals such that

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Another need for interval arithmetic comes from the roundoff errors that occur when working with finite precision numbers.

Notable applications of interval arithmetic to bring rigor to numerical computations performed on a computer include:

- T. Hales' proof of Kepler's conjecture (see https://code.google.com/p/flyspeck/),
- W. Tucker's solution of Smale's 14th problem (see https://www2.math.uu.se/~warwick/main/thesis.html and also https://paulbourke.net/fractals/lorenz/).

Numerous additional interesting information on the website https://www.cs.utep.edu/interval-comp/.

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Note that, in practice, one commonly uses relative error  $\left|1 - \frac{\widehat{f(x)}}{\widehat{f(x)}}\right|$  rather than absolute error  $|\widehat{f(x)} - f(x)|$ .

We focus on the absolute error case for the sake of clarity.

To perform the evaluation, we replace f by a polynomial p. Then we evaluate p, and  $\widehat{f(x)} = \circ(p(x))$ , where  $\circ$  is the active rounding mode.

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There are two sources of error:

- approximation error: let  $\eta_1$  be an upper bound for  $\|f p\|_{\infty}$ ,
- rounding error: let  $\eta_2$  be an upper bound for the error  $|p\left(x
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  ight)|$ ,

we have to guarantee that  $\eta_1 + \eta_2 \leqslant \varepsilon$ .

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we have to guarantee that  $\eta_1 + \eta_2 \leq \varepsilon$ .

In this course: tools that help to establish rigorous approximation error.

Regarding rounding errors, G.Melquiond has developed formal proof tools (in Coq) which address this issue (see https://gappa.gitlabpages.inria.fr/).

## Definition

(Real interval.) Let  $\bar{x}, \underline{x} \in \mathbb{R}$ ,  $\bar{x} \leq \underline{x}$ . We define the interval

 $X = [\underline{x}, \overline{x}] = \{x \in \mathbb{R} : \underline{x} \leqslant x \leqslant \overline{x}\}.$ 

The real numbers  $\underline{x}$  and  $\overline{x}$  are called the endpoints of the interval,  $\underline{x}$  is its minimum,  $\overline{x}$  its maximum. The set of all real intervals will be denoted  $\mathbb{IR}$ .

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#### Definition

Let  $x \in \mathbb{IR}$ . The width of x is denoted  $w(x) = \overline{x} - \underline{x}$ . We also define the center

$$\operatorname{mid}\left(x\right) = \frac{\underline{x} + x}{2},$$

and the radius  $rad(x) = \frac{1}{2}w(x)$ .

### Remark

It is common in the litterature to encounter the notation  $(\operatorname{mid}(x), \operatorname{rad}(x)) = \{x \in \mathbb{R} : |x - \operatorname{mid}(x)| \leq \operatorname{rad}(x)\}.$ 

This mid-rad representation is the basis of the so called Ball Arithmetic, cf. the excellent software Arb, now a part of FLINT https://flintlib.org/.

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## Definition

A point (or degenerate, or thin) interval is one of the form [x, x], also denoted [x].

We now define basic arithmetic operations on intervals. As you will see, monotonicity plays an essential role for obtaining sharp enclosures.

#### Definition

Let  $X, Y \in \mathbb{IR}$ . Let  $* \in \{+, -, \times, /\}$ . We denote

$$X * Y = \{x * y; x \in X, y \in Y\}$$

where, if \* = /, we assume that  $0 \notin Y$ .

## 3.1.1. Operations on intervals

## Proposition

We can compute the X \* Y above using formulae such as

$$\begin{split} & [\underline{x}, \bar{x}] + [\underline{y}, \bar{y}] = [\underline{x} + \underline{y}, \bar{x} + \bar{y}], \\ & [\underline{x}, \bar{x}] - [\underline{y}, \bar{y}] = [\underline{x} - \bar{y}, \bar{x} - \underline{y}], \\ & [\underline{x}, \bar{x}] \times [\underline{y}, \bar{y}] = [\min\left(\underline{x} \cdot \underline{y}, \underline{x} \cdot \bar{y}, \bar{x} \cdot \underline{y}, \bar{x} \cdot \bar{y}\right), \max\left(\underline{x} \cdot \underline{y}, \underline{x} \cdot \bar{y}, \bar{x} \cdot \underline{y}, \bar{x} \cdot \bar{y}\right)], \\ & [\underline{x}, \bar{x}] / [\underline{y}, \bar{y}] = [\underline{x}, \bar{x}] \times \left[\frac{1}{\bar{y}}, \frac{1}{\underline{y}}\right] \quad \text{if } 0 \notin Y, \end{split}$$

which depend only on the endpoints.



## 3.1.1. Operations on intervals

#### Remark

Note that, in  $\mathbb{IR},$  the operations + and  $\times$  are associative and commutative.

### Remark

In practice, multiplication (hence division) can be made more efficient (check the signs of the endpoints).

## 3.1.1. Operations on intervals

### Proposition

- Interval subtraction is not the inverse of addition.
- Interval division is not the inverse of multiplication.
- **③** Interval multiplication of an interval with itself is not equivalent to "squaring the interval": if  $\underline{x} < 0 < \overline{x}$ ,

$$[\underline{x}, \overline{x}] \times [\underline{x}, \overline{x}] \neq \left[0, \max\left(\underline{x}^2, \overline{x}^2\right)\right].$$

Interval multiplication is sub-distributive wrt addition: for all X, Y, Z ∈ Iℝ, we have

$$X \times (Y+Z) \subset X \times Y + X \times Z.$$

**5** For all  $X \in \mathbb{IR}$ , we have X + [0] = X and  $[0] \times X = [0]$ .

#### Proof.

Exercise.

## A straightforward yet quite useful statement is the following.

#### Lemma

(Inclusion isotonicity) If  $X \subset X', Y \subset Y', * \in \{+, -, \times, /\}$ , then

 $X * Y \subset X' * Y'.$ 

For division, we assume that  $0 \notin Y'$ .

#### Proof.

Obvious from Definition .

## 3.1.2. Floating-point interval arithmetic

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When we perform arithmetic operations on intervals in  $\mathbb{IF}$ , we need to make sure to "round the resulting interval outwards" in order to guarantee that it contains the "true result".

## For $X,Y\in\mathbb{I}\mathcal{F},$ we set

$$\begin{split} X+Y &= \left[ \nabla \left(\underline{x}+\underline{y}\right), \bigtriangleup \left(\bar{x}+\bar{y}\right) \right], \\ X-Y &= \left[ \nabla \left(\underline{x}-\bar{y}\right), \bigtriangleup \left(\bar{x}-\underline{y}\right) \right], \\ X\times Y &= \left[ \min \left( \nabla \left(\underline{x}\underline{\cdot}\underline{y}\right), \nabla \left(\underline{x}\underline{\cdot}\bar{y}\right), \nabla \left(\bar{x}\underline{\cdot}\underline{y}\right), \nabla \left(\bar{x}\underline{\cdot}\bar{y}\right) \right), \\ \max \left( \bigtriangleup \left(\underline{x}\underline{\cdot}\underline{y}\right), \bigtriangleup \left(\underline{x}\underline{\cdot}\bar{y}\right), \bigtriangleup \left(\bar{x}\underline{\cdot}\underline{y}\right), \bigtriangleup \left(\bar{x}\underline{\cdot}\bar{y}\right) \right) \right], \\ X/Y &= \left[ \min \left( \nabla \left(\underline{x}/\underline{y}\right), \nabla \left(\underline{x}/\bar{y}\right), \nabla \left(\bar{x}/\underline{y}\right), \nabla \left(\bar{x}/\bar{y}\right) \right), \\ \max \left( \bigtriangleup \left(\underline{x}/\underline{y}\right), \bigtriangleup \left(\underline{x}/\bar{y}\right), \bigtriangleup \left(\bar{x}/\underline{y}\right), \bigtriangleup \left(\bar{x}/\bar{y}\right) \right) \right], \\ \max \left( \bigtriangleup \left(\underline{x}/\underline{y}\right), \bigtriangleup \left(\underline{x}/\bar{y}\right), \bigtriangleup \left(\bar{x}/\bar{y}\right), \bigtriangleup \left(\bar{x}/\bar{y}\right) \right) \right] \quad if \ 0 \notin Y, \end{split}$$

where  $\triangledown$  and  $\triangle$  denote rounding to  $-\infty$  and  $+\infty$  respectively.

# 3.1.2. Floating-point interval arithmetic

#### Remark

Standard machine floating-point numbers are not always sufficient, e.g., to work with very small intervals. We may also use multiple-precision floating-point numbers as bounds for our intervals. An example of a library which offers support for multiple precision interval arithmetic is  $MPFR^1$ .

<sup>&</sup>lt;sup>1</sup>http://www.mpfr.org

## 3.2. Interval functions

## Definition

Let  $D \subset \mathbb{R}$ , and let  $f : D \to \mathbb{R}$ . We denote

 $R(f,D) = \{f(x) : x \in D\}$ 

the range of f over D.

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#### Remark

Finding the exact image of a (usually multivariate) function, and, in particular, a value where f attains its minimum is a whole subdomain of Math and CS called Global Optimization.

Let  $X = [\underline{x}, \overline{x}] \in \mathbb{IR}$ . By monotonicity, interval functions defined as follows give the exact range of the corresponding real functions:

$$e^{X} = [\exp \underline{x}, \exp \overline{x}],$$
$$\sqrt{X} = \left[\sqrt{\underline{x}}, \sqrt{\overline{x}}\right], \qquad \underline{x} \ge 0,$$
$$\log X = \left[\log \underline{x}, \log \overline{x}\right], \qquad \underline{x} > 0,$$
$$\arctan X = \left[\arctan \underline{x}, \arctan \overline{x}\right],$$

For some other functions like  $x^n$ , trigonometric functions..., writing down R(f, D) is also possible, as long as we know their extrema. For instance, let  $n \in \mathbb{Z}$ ,  $X \in \mathbb{IR}$ ,

$$X^{n} = \operatorname{pow}\left(X, n\right) = \begin{cases} \operatorname{if} n \in 2\mathbb{N} + 1, [\underline{x}^{n}, \overline{x}^{n}] \\ \operatorname{if} n \in \mathbb{N} \setminus \{0\}, n \operatorname{even}, \\ [\min\left(\underline{x}^{n}, \overline{x}^{n}\right), \max\left(\underline{x}^{n}, \overline{x}^{n}\right)] \operatorname{if} 0 \notin X, \\ [0, \max\left(\underline{x}^{n}, \overline{x}^{n}\right)] \operatorname{otherwise}, \\ [1, 1] \operatorname{if} n = 0, \\ [1/\overline{x}, 1/\underline{x}]^{-n} \operatorname{if} - n \in \mathbb{N} \operatorname{and} 0 \notin X. \end{cases}$$

## 3.2. Interval functions

## Exercise

Write the analogous formulas for sin, cos, tan. For sin and tan, consider

$$S_1^+ = \left\{ 2k\pi + \frac{\pi}{2}, k \in \mathbb{Z} \right\}, \quad S_1^- = \left\{ 2k\pi - \frac{\pi}{2}, k \in \mathbb{Z} \right\}.$$

For cos, consider

$$S_2^+ = \{2k\pi, k \in \mathbb{Z}\}, \quad S_2^- = \{2k\pi + \pi, k \in \mathbb{Z}\}.$$

The example of  $f\left(x\right)=x^{2}-x+1$  over  $\left[0,2\right]$  illustrates two important issues:

- overestimation;
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Actually, R(f, [0, 2]) = [3/4, 3].