Approximation of functions

We want a formula

We know:

- the function in full (at any point by a slow method)
- values (sometimes also derivatives) at discrete points

Quality of data:

- arbitrary precision
- approximate (experiment, simulation)

Methods:

- Taylor (McLaurin) / Padé (rational function), Thiele
- interpolation
- splines
- orthogonal systems of functions
- Chebyshev (best) approximation
- least square method – fitting, correlation, regression

Taylor (MacLaurin)

MacLaurin (shifted $x = 0 \to x = x_0$ = Taylor)
All derivatives must be known, in $\mathbb{R}$, $\mathbb{C}$, . . . :

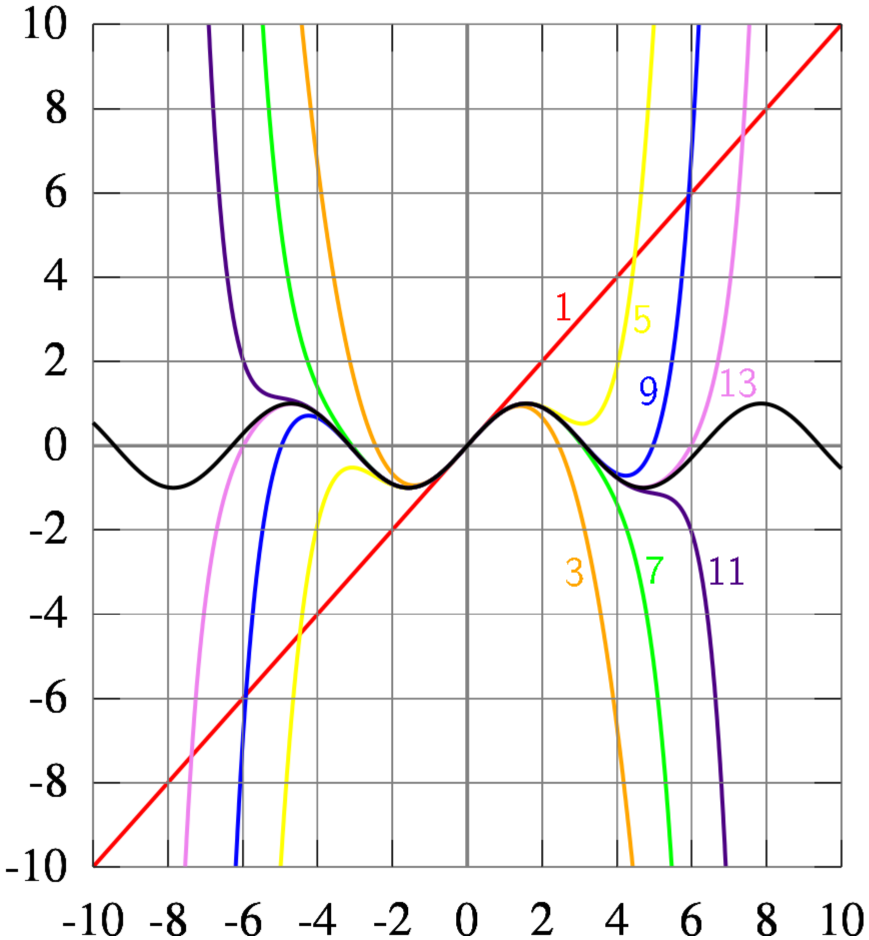
$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} x^n$$

- accurate close to $x = 0$
- the larger x, the less accurate
- convergence not guaranteed, e.g.:

$$f(x) = \begin{cases} \exp(-1/x) & \text{for } x > 0, \\ 0 & \text{for } x \le 0 \end{cases}$$

is smooth (all derivatives at $x = 0$ are zero), but not analytic (zero radius of convergence of the Taylor series)

Example. Study the convergence (partial sums) of the Taylor series of function $\sin(x)$ at $x = 0$.



credit: Wikipedia

Padé

The Padé approximation of function $f(x)$ at $x = 0$ is the rational function:

$$f(x) \approx \frac{P_k(x)}{P_{n-k}(x)}, \quad P_l(x) = \sum_{i=0}^{l} a_i x^i$$

which has the same derivatives as f at 0 up to $f^{(n)}(0)$ (i.e., the same Taylor expansion)

Accurate close to $x = 0$, inaccurate for large x

Often (but not always) more accurate than Taylor of the same order

Calculation:

- Taylor-expand both sides of the equation and compare the coefficients
- Use the Thiele theorem for the continued fraction

Application:

- Speed up the convergence, e.g., of the virial equation of state

Continued fraction

Equivalent expression for the rational function

E.g.:

$$a_0 + \frac{x}{a_1 + \frac{x}{a_2 + \frac{x}{a_3}}} = a_0 + \frac{x\,|}{|a_1} + \frac{x\,|}{|a_2} + \frac{x\,|}{|a_3}$$

Infinite continued fraction (example):

$$\arctan x = \frac{x|}{|1} + \frac{1^2x^2|}{|\;\;3} + \frac{2^2x^2|}{|\;\;5} + \frac{3^2x^2|}{|\;\;7} + \cdots \quad \text{converges for } x \in \mathbb{R}$$

Taylor expansion:

$$\arctan x = x - \frac{x^3}{3} + \frac{x^5}{5} - + \cdots \quad \text{converges for } x \le 1$$

Evaluations

Evaluate a polynomial (direct):

$$P_n(x) = \sum_{i=0}^{n} a_n x^n = a_0 + x(a_1 + x(a_2 + \ldots)) \quad n \text{ multiplications and } n \text{ additions}$$

NB: P_4 can be evaluated in 3 multiplications and 5 additions, P_5 in 4 multiplications and 5 additions

Continued fraction (recursive):

$$f_n = a_0 + \frac{b_1 \mid}{\mid a_1} + \frac{b_2 \mid}{\mid a_2} + \cdots + \frac{b_n \mid}{\mid a_n}$$

algorithm for any n:

$$\begin{aligned} A_{-1} &:= 0, & B_{-1} &:= 1 \\ A_0 &:= 1, & B_0 &:= a_0 \\ A_j &:= a_j A_{j-1} + b_j A_{j-2}, & B_j &:= a_j B_{j-1} + b_j B_{j-2}, \quad j = 1..n \end{aligned}$$

$$f_n = \frac{B_n}{A_n}$$

NB: A_j, B_j may overflow, there are methods avoiding this

Thiele theorem

for continued fractions is analogous to Taylor for polynomials.

$$f(x) = f(0) + \frac{x\ |}{|r_1(0)} + \frac{x\ |}{|r_2(0)} + \frac{x\ |}{|r_3(0)} + \cdots$$

where recursively:

$$\begin{aligned} R_{-1} &= 0 \\ R_0 &= f(x) \\ R_j(x) &= R_{j-2}(x) + r_{j-1}(x) \\ r_j(x) &= \frac{j+1}{R_j'(x)} \end{aligned}$$

Example: $\ln(1+x)$

$$\begin{aligned} R_0 &= ln(1+x) \\ r_0 &= 1/(1/(1+x)) = 1 + x \overset{x=0}{=} \boxed{1} \\ R_1 &= R_{-1} + r_0 = 1 + x \\ r_1 &= 2/(1+x)' = \boxed{2} \\ R_2 &= R_0 + r_1 = \ln(1+x) + 2 \\ r_2 &= \frac{3}{1/(1+x)} = 3(1+x) \overset{x=0}{=} \boxed{3} \\ &\vdots \end{aligned}$$

$$r_{2n} = 2n + 1,\ r_{2n+1} = 2/(n+1)$$

$$\ln(1+x) = \frac{x|}{|1} + \frac{x\ |}{|2/1} + \frac{x|}{|3} + \frac{x\ |}{|2/2} + \frac{x|}{|5} + \frac{x\ |}{|2/3} + \cdots$$

Approximation by orthogonal functions

Let $b_n(x)$ be a complete system (basis) of real orthonormal functions in interval $[a, b]$. Then (in some sense of convergence. . .)

$$f(x) = \sum_{i=0}^{\infty} a_i b_i(x), \quad \text{where } a_n = \int_a^b f(x) b_n(x) \mathrm{d}x$$

Let us denote the partial sum as $f_n(x) = \sum_{i=0}^{n} a_i b_i(x)$

Then the coefficients a_i minimize the following "error" of the approximation (integral of squares of the deviations):

$$\int_a^b |f_n(x) - f(x)|^2 \mathrm{d}x \tag{1}$$

Notes:

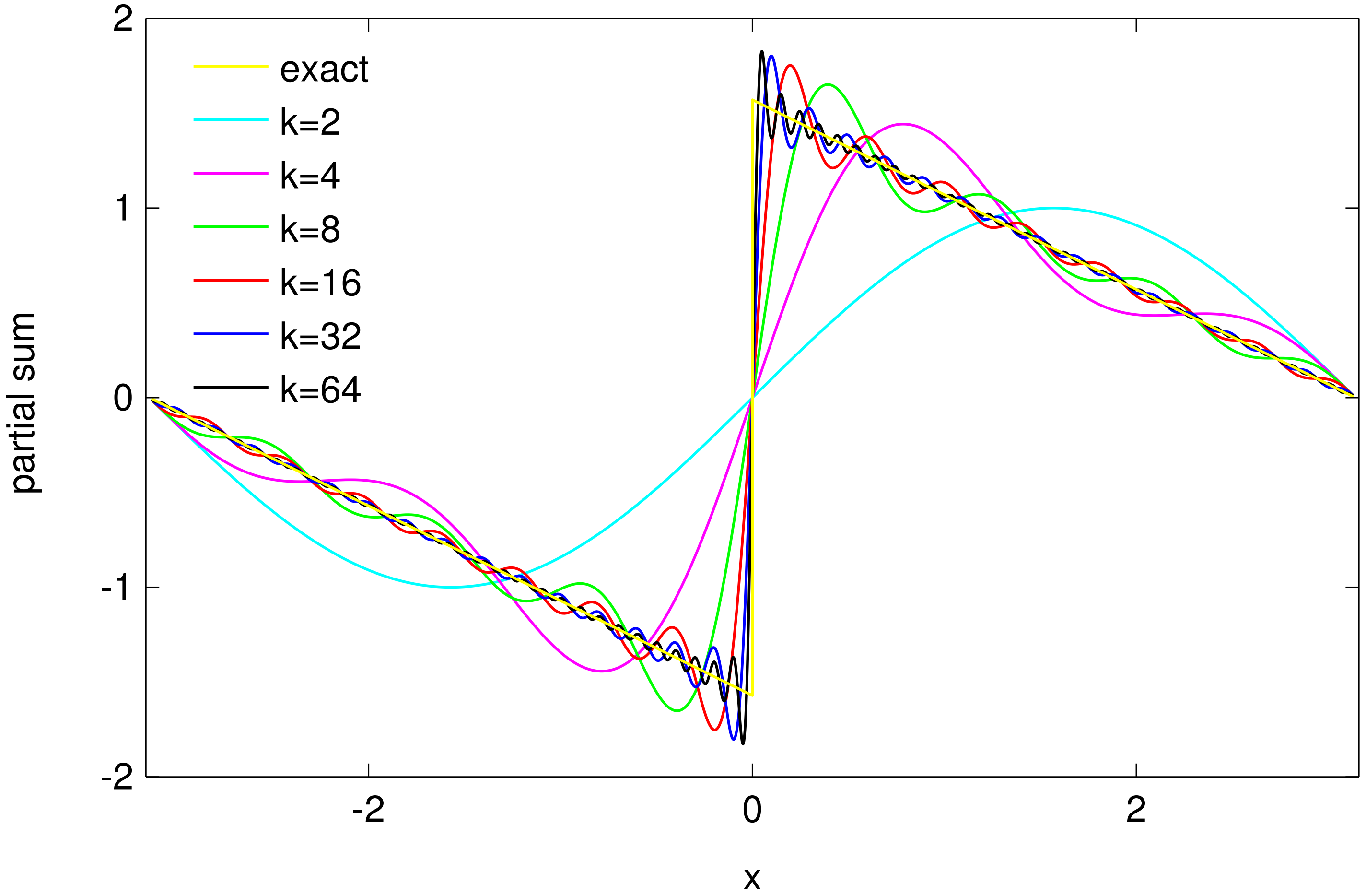
- To approximate certain classes of decaying functions, an unbounded interval can be considered, cf. `mat-lin2.mw`.
- Scalar product with a weight can be used (see, e.g., Chebyshev)

Example – Fourier series

Fourier series for functions $f(x), x \in [0, 2\pi]$, such that $\int_0^{2\pi} |f^2| dx$ exists:

- basis = $\{1, \sin x, \cos x, \sin 2x, \cos 2x \ldots\}$
- good for "smooth enough" periodic functions
- limited advantage for numerical purposes (slow sin, cos)

$$\sum_{i=1}^{k} \frac{\sin(ix)}{i}$$



Approximation by orthogonal functions

Let-us orthogonalize functions $\{1, x, x^2, \ldots\}$ at interval $[-1, 1]$ by the Gram-Schmidt method. The resulting set of orthogonal polynomials is called **Legendre polynomials** (see `matenum1.mw`).

- least-square-type approximation (minimizes (1))
- larger deviations near the interval ends

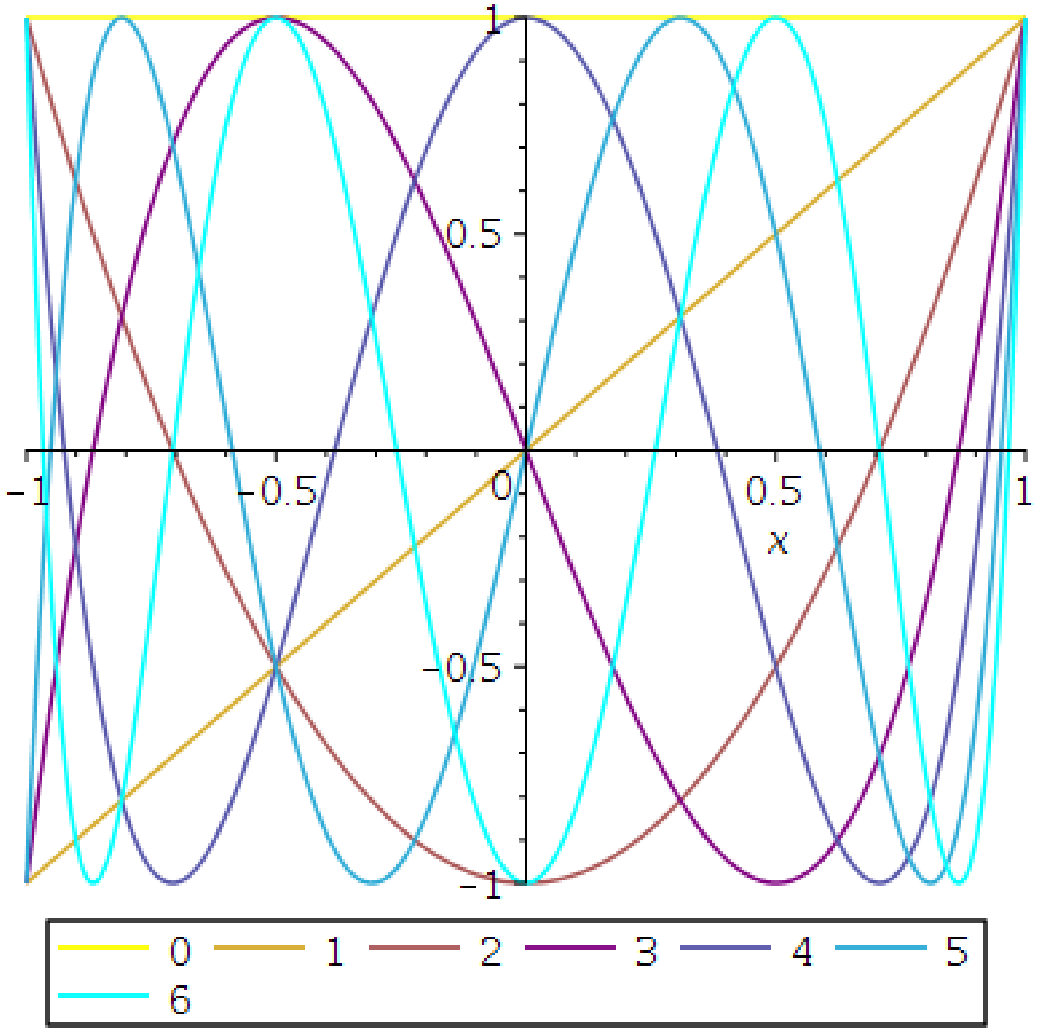
Chebyshev polynomials are often better

English: Pafnuty Lvovich Chebyshev   Russian: Пафну́тий Льво́вич Чебышёв
Czech: Pafnutij Lvovič Čebyšov (often incorrectly Čebyšev)

Orthogonal in interval $[-1,1]$ with weight $1/\sqrt{1-x^2}$

$$T_n(x) = \cos(n \arccos x)$$

$$\int_{-1}^{1} \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}} \mathrm{d}x = \begin{cases} 0 & \text{for } n \neq m \\ \pi & \text{for } n = m = 0 \\ \pi/2 & \text{for } n = m \neq 0 \end{cases}$$



The expansion:

$$f(x) \approx \frac{c_0}{2} + \sum_{i=1}^{n} c_i T_n(x)$$

$$c_i = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x)T_n(x)}{\sqrt{1-x^2}} \mathrm{d}x = \frac{2}{\pi} \int_{-\pi/2}^{\pi/2} f(\sin\theta) T_n(\sin\theta) \mathrm{d}\theta$$

- close to the best (minimax) approximation

mmpc3.mw: Chebyshev 2×

The Chebyshev best (minimax) approximation

= the approximation which minimizes the maximum deviation:

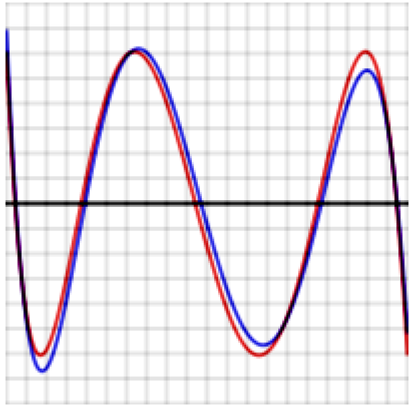
$$\min_{a_i}[\max_x |f(x) - P_n(x)|]$$

where $P_n(x) = \sum_{i=0}^{n} a_i x^i$ is a polynomial with $n+1$ coefficients

- The best approximation always exists
- The deviation $f(x) - P_n(x)$ has:
  – $n+2$ extremes, with alternating maxima and minima
  – $n+1$ zero points
  – the expansion by Chebyshev polynomials is usually quite close to it

Similar statement for a rational function (of $n+1$ independent parameters).

Example: $\ln(x)$ in interval $[2,4]$ approximated by the Chebyshev polynomials (—) and the best approximation (—); the deviation is shown.



credit: Wikipedia

Interpolation

A function is known at discrete points, (x_i, y_i), $i = 1..n$.
We want a polynomial coinciding with these points.
There is a unique polynomial of the order $n-1$ (to x^{n-1})
= **Lagrange interpolation polynomial**:

$$
\begin{aligned}
y(x) \quad = \quad & y_1 \frac{\cancel{(x_1-x)}(x_2-x)(x_3-x)\cdots(x_n-x)}{\cancel{(x_1-x_1)}(x_2-x_1)(x_3-x_1)\cdots(x_n-x_1)} \\
+ \quad & y_2 \frac{(x_1-x)\cancel{(x_2-x)}(x_3-x)\cdots(x_n-x)}{(x_1-x_2)\cancel{(x_2-x_2)}(x_3-x_2)\cdots(x_n-x_2)} \\
\vdots \quad & \\
+ \quad & y_n \frac{(x_1-x)(x_2-x)(x_3-x)\cdots\cancel{(x_n-x)}}{(x_1-x_n)(x_2-x_n)(x_3-x_n)\cdots\cancel{(x_n-x_n)}}
\end{aligned}
$$

- Can be simplified for equidistant x's
- May be inaccurate close to endpoints for equidistant subintervals
- Can be extended if also derivatives are known

mmpc3.mw: Interpolation by a polynomial and a rational function

Splines

A function is known at discrete points, (x_i, y_i), $i = 0..n$.
We want a set of polynomials piecewise in intervals $[x_i, x_{i+1}]$.
The most common cubic splines: (total $4n$ constants):

- coincide at points (x_i, y_i) ($2n$ conditions)
- continuous derivatives ($n - 1$ conditions)
- continuous 2nd derivatives ($n - 1$ conditions)

There are 2 conditions for the coefficients left. We may demand zero 2nd derivatives at the ending points, or to minimize the squared deviation of maximum error

If we know the 1st derivatives, we may want to reproduce them; then, we must resign to continuous 2nd derivatives (or increase the order).

- Useful to approximate a complex function on a computer (e.g., interaction of Gaussian charges)

pros: simple to obtain
a few floating point operations
cons: calculation of an integer i required (may be slow)
tables need not fit into a cache