Note: The discrete Chebyshev expansion that results from use of the trapezoidal integration in the θ variable

$$f(x) \sim \sum_{k=0}^{n} \tilde{a}_k T_k(x) \qquad (3)$$

is interpolatory:

$$f(x_j) = \sum_{k=0}^{n} \tilde{a}_k T_k(x_j)$$

Clearly, the right-hand side of (3) is a polynomial of degree n. That is to say, the polynomial interpolant to a function f at the Chebyshev interpolation points

equispaced

$x_j = \cos(\theta_j)$ converges to f!

(Unlike in the case x_j equispaced.)

Before actually describing the computational applications of Chebyshev expansions, we place them in a much broader context related to Sturm-Liouville theory

Sturm–Liouville context

The trigonometric expansions inherent in the Chebyshev approximations arose from the simple Sturm–Liouville problem

$$\frac{d^2 e}{d\theta^2}(\theta) + k^2 e(\theta) = 0 \qquad (4)$$

We can re-state this problem in the x-variable.

Noting that

$$\frac{d}{d\theta} = -\sin(\theta)\frac{d}{dx} = -\sqrt{1-x^2}\,\frac{d}{dx}$$

$$\frac{d^2\theta}{d\theta^2} = \frac{d}{d\theta}\left(\frac{d\theta}{d\theta}\right) =$$

$$= -\sqrt{1-x^2}\,\frac{d}{dx}\left[-\sqrt{1-x^2}\left(\frac{dT}{dx}\right)\right],$$

The eigenvalue equation (4) becomes

the (singular) Sturm-Liouville equation

$$\frac{d}{dx}\left[\underbrace{\sqrt{1-x^2}}_{p}\left(\frac{dT}{dx}\right)\right] + \overbrace{k^2}^{\lambda}\,\underbrace{\frac{1}{\sqrt{1-x^2}}}_{\rho}\,T = 0$$

$$(q = 0).$$

A similar equation is obtained e.g. in the process

of separation of variables for the Laplace equation in the sphere. Indeed, the equation that results in that case for the polar angle is usually expressed in the form

$$\frac{d}{dx}\left[(1-x^2)\left(\frac{dP}{dx}\right)\right] - \frac{m^2}{(1-x^2)}P + \lambda P = 0 .$$

For $m=0$ the solutions are the "Legendre polynomials". For $m \neq 0$ they are the "associated Legendre functions" (not polynomials). These are complete systems for each integer m (per theory presented previously.)

We have thus considered the Sturm-Liouville problems

k^2

$$\frac{d}{dx}\left[\sqrt{1-x^2}\left(\frac{dT_k}{dx}\right)\right] + \lambda \frac{1}{\sqrt{1-x^2}} T_k = 0$$

and

$$\frac{d}{dx}\left[(1-x^2)\left(\frac{dP_k}{dx}\right)\right] + \lambda P_k = 0$$

$k(k+1)$ (can show)

One way to see that the solutions must be polynomials is by first showing that the left-hand operators, for any given λ, map a polynomial of any given degree into a polynomial of the same degree.

(In the Chebyshev case it is useful to first re-express the equation in the form

$$(1-x^2)\frac{d^2T}{dx^2} - x\frac{dT}{dx} + \lambda T = 0.$$

Can generalize! The calculations yield the same results for an equation of the form

$$(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d}{dx}\left[(1-x)^{\alpha+1}(1+x)^{\beta+1}\frac{dJ}{dx}\right)\Big] + \lambda J$$

$$= 0.$$

Jacobi polynomials! Complete!

Particular cases: Chebyshev, Legendre, Gegenbauer ($\alpha=\beta$).

Fast/Slow convergence

Whether polynomial or not, some SL expansions converge fast (e.g. Chebyshev) whereas others do not (e.g. Bessel).

In what follows we study this phenomenology.

Do Legendre expansions converge fast?

How about Jacobi?

How about a general (singular or regular) Sturm-Liouville problem

$$(p\phi')' - q\phi + \lambda w \phi = 0 \qquad a < x < b \qquad (5)$$

(We assume the coefficients p, q and w satisfy the conditions for completeness studied previously.)

(We follow Gottlieb and Orszag.)

We assume the eigenfunctions have been normalized:

$$\int_a^b \phi_n^2 \, w(x)\, dx = 1,$$

and we consider non-singular problems first:

$$\left.\begin{array}{l} p>0,\ w>0 \\ p,\ q,\ w \ \text{smooth} \end{array}\right\} \text{ for } a \le x \le b$$

The coefficients a_n in the eigenfunction expansion

$$f(x) = \sum_{n=1}^{\infty} a_n \phi_n(x)$$

are given by

$$a_n = \int_a^b f(x)\,\underline{\phi_n(x)\,w(x)}\,dx.$$

Substituting the SL equation (5) with $\phi = \phi_n$ and $\lambda = \lambda_n$ we obtain

$$a_n = \frac{1}{\lambda_n}\int_a^b \left(-(p\phi_n')' + q\,\phi_n\right) f(x)\,dx.$$

Integrating by parts twice we obtain

$$a_n = \frac{1}{\lambda_n}\Big[p(x)\left[\phi_n(x) f'(x) - \phi_n'(x) f(x)\right]\Big]_{x=a}^{x=b}$$

$$+ \frac{1}{\lambda_n}\int_a^b \left[(-pf')' + qf\right]/w \cdot \phi_n\, w\, dx$$

We consider the case of the boundary conditions $\phi(a) = \phi(b) = 0$

It follows that

$$a_n = \underbrace{\frac{1}{\lambda_n}}_{\sim n^2} \left[p(a)\, \overbrace{\phi_n'(a)}^{\sim n} f(a) - p(b)\, \overbrace{\phi_n'(b)}^{\sim n} f(b) \right] + O\left(1/\lambda_n\right) \qquad (6)$$

(since the integral term is the Fourier coefficient of a regular function).

As we know $\lambda_n \longrightarrow \infty$ as $n \longrightarrow \infty$.

From (6) it follows that if the bracket does not vanish.

The eigenvalues generally tend to infinity like $\lambda_n \sim O(n^2)$. Taking into account also the values of ϕ_n' (see G+O) it follows that

$$a_n \sim \mathcal{O}(1/n),$$

and not better. This results in slow decay and Gibbs phenomenon. (It can be shown that

$$\phi_n \sim A_n \sin\left(\sqrt{\lambda_n}\int_a^x \sqrt{\frac{w}{p}}\,dx\right),$$

see references in G+O.)

Generically, the Fourier expansions for non-singular SL problems have $a_n \sim \mathcal{O}\left(\frac{1}{n}\right)$. We have seen that, under such conditions, the Gibbs phenomenon is observed. Whether the Gibbs phenomenon occurs in a particular example, depends on the actual boundary values of the functions f, ϕ_n, ϕ_n' and p, which may lead, in some cases, to a vanishing numerator in (6).

Examples

Bessel functions of order $\nu=0$.

$$(x\phi_n')' + \lambda_n x \phi_n = 0$$

$$\phi_n(0) \text{ finite}, \quad \phi_n(1) = 0.$$

We have $p(x) = w(x) = x$. The problem is singular at $x=0$, but nonsingular at $x=1$. The eigenfunctions are

$$\phi_n(x) = J_0(j_{0n}\, x)$$

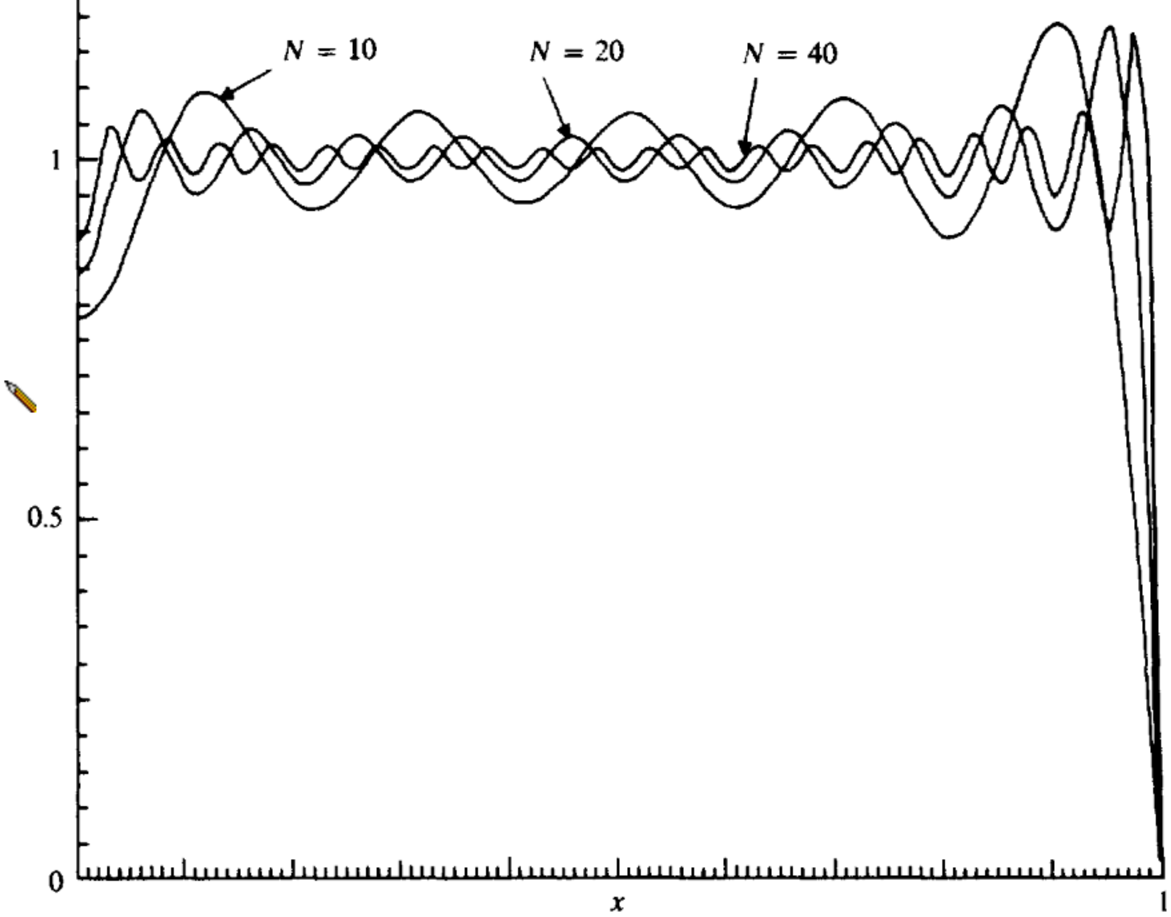
where J_0 is the Bessel function of order zero.

The eigenvalues are $\lambda_n = j_{0n}$ satisfy

$$j_{0n} \sim (n - 1/4)\pi$$

slow convergence (but no Gibbs) at $x=0$.

Gibbs phenomenon: overshoot (does not tend to zero).



Bessel J_0 expansion of the function 1.

With some additional analysis it can be shown that there is convergence at zero, but with an error of the order $O(N^{1/2})$.

How about Legendre polynomials, or, more generally, Jacobi polynomials. For Chebyshev polynomials, another subclass of the Jacobi polynomials, we know that fast convergence takes place.

To study this problem we consider equation (6).

In the Jacobi case we have $p(a) = p(b) = 0$.

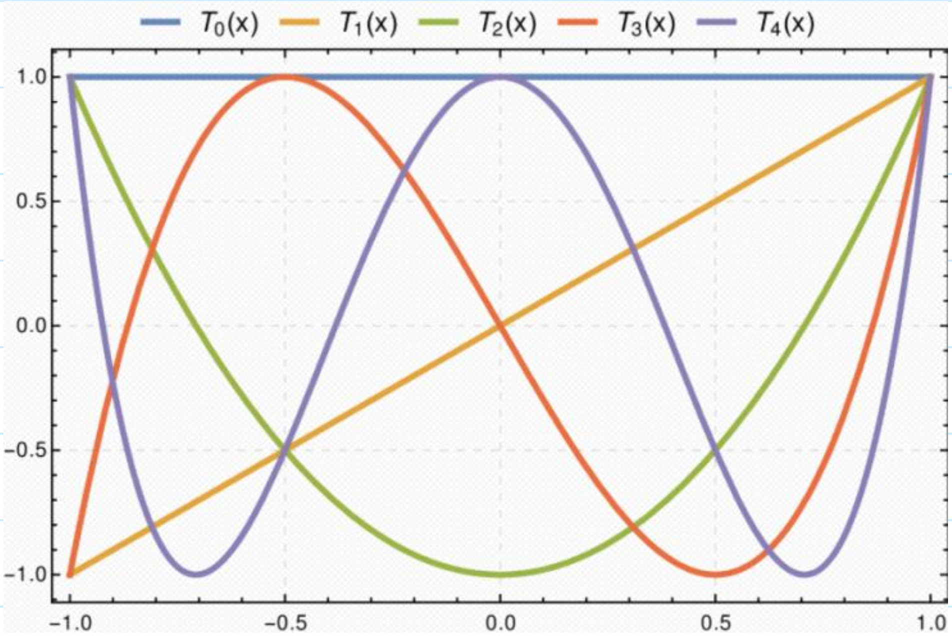
It can be shown that we can integrate by parts as many times as desired, (limited only by the smoothness of the function f). For infinitely smooth f, convergence of order $O(N^{-p})$ for all positive intergers p (also called "superalgebraic" convergence) is achieved.

Chebyshev expansions

Practical Implementation

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

$T_n(x)$ is a polynomial of degree n



$$
\begin{aligned}
T_0(x) &= 1 \\
T_1(x) &= x \\
T_2(x) &= 2x^2 - 1 \\
T_3(x) &= 4x^3 - 3x \\
T_4(x) &= 8x^4 - 8x^2 + 1 \\
T_5(x) &= 16x^5 - 20x^3 + 5x \\
T_6(x) &= 32x^6 - 48x^4 + 18x^2 - 1 \\
T_7(x) &= 64x^7 - 112x^5 + 56x^3 - 7x \\
T_8(x) &= 128x^8 - 256x^6 + 160x^4 - 32x^2 + 1 \\
T_9(x) &= 256x^9 - 576x^7 + 432x^5 - 120x^3 + 9x \\
T_{10}(x) &= 512x^{10} - 1280x^8 + 1120x^6 - 400x^4 + 50x^2 - 1 \\
T_{11}(x) &= 1024x^{11} - 2816x^9 + 2816x^7 - 1232x^5 + 220x^3 - 11x
\end{aligned}
$$

$$u(\cos(\theta)) = \sum_n \hat{u}_n \cos(n\theta)$$

$$u(x) = \sum_n \hat{u}_n \cos(n \arccos(x)).$$

$$u(x) = \sum_n \hat{u}_n T_n(x)$$

Discrete Chebyshev expansions can be obtained by exploiting the discrete methods, based on use of trapezoidal quadrature, for trigonometric Fourier expansions

The resulting expressions are given in what follows for three different kinds of equispaced discretizations.

To do this recall the expression

$$\hat{u}_n = \frac{2}{\pi c_n} \int_0^{\pi} u(\cos(\theta)) \cos(n\theta) \, d\theta .$$

$(c_0 = 2$ and $c_n = 1$ for $n > 0)$.

We can apply the trapezoidal rule in several ways, namely, including either both endpoints, or just one endpoint, or no endpoints.

These are known by proper names, and listed in what follows.

- Chebyshev – Gauss (open – open)

$$\theta_j = \frac{(2j+1)\pi}{2N+2}, \quad w_j = \frac{\pi}{N+1} \qquad 0 \le j \le N$$

- Chebyshev Gauss–Lobatto (closed – closed)

$$\theta_j = \frac{j\pi}{N}, \qquad w_j = \frac{\pi}{\tilde{c}_j N}, \quad 0 \le j \le N$$

$(\tilde{c}_0 = \tilde{c}_N = 2$ and $\tilde{c}_j = 1$ for $j = 1, \cdots, N-1)$.

- Chebyshev Gauss–Radau (closed – open)

$$\theta_j = \frac{2\pi j}{2N+1}, \qquad 0 \le j \le N$$

$$w_0 = \frac{\pi}{2N+1}, \quad w_j = \frac{2\pi}{2N+1} \qquad (1 \le j \le N)$$

Note that the points $x_j = \cos(\theta_j)$ are clustered in a neighborhood of ± 1 For example in the CGL case we have

$$1-x_1 = 1-\cos\left(\frac{\pi}{N}\right) = 2\sin^2\frac{\pi}{2N} \sim \frac{\pi^2}{2N^2} \quad (N \gg 1).$$

Using these points we obtain expressions for approximate coefficients and associated Chebyshev interpolants. In all cases we have

$$\boxed{\tilde{u}_n = \frac{2}{\pi c_n}\sum_{j=0}^{N} u(x_j)\cos(n\theta_j)\,\omega_j}$$

In the CGL case, for example, we obtain

$$\tilde{u}_n = \frac{2}{\tilde{c}_n N}\sum_{j=0}^{N}\frac{1}{\tilde{c}_j}\,u(x_j)\cos\left(\frac{nj\pi}{N}\right)$$

$$0 \le j \le N$$

and

$$(I_N u)(x) = \sum_{n=0}^{N}\tilde{u}_n T_n(x).$$

Differentiation matrix (CGL case)

(Trefethen, p.53)

$$x_j = \cos(j\pi/N), \quad j = 0, 1, \dots, N$$

Given the vector

$$U = (u(x_0), u(x_1), \dots, u(x_N))^t,$$

the vector

$$V = D_N U$$

contains the values of the derivatives of $(I_N u)$, respect to x, at the points $x_0, x_1, \dots, x_N$. The matrix D_N is given by

$$(D_N)_{00} = \frac{2N^2+1}{6}, \qquad (D_N)_{NN} = -\frac{2N^2+1}{6},$$

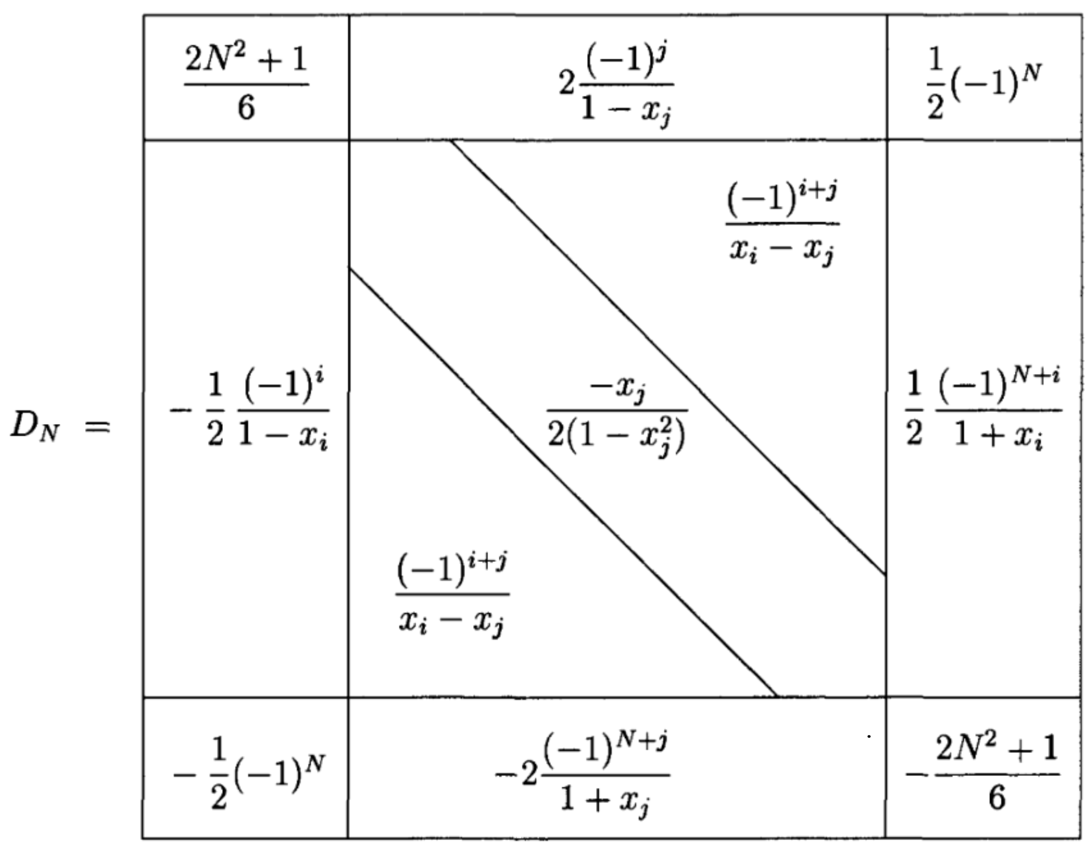
$$(D_N)_{jj} = \frac{-x_j}{2(1-x_j^2)}, \qquad j = 1, \ldots, N-1,$$

$$(D_N)_{ij} = \frac{c_i}{c_j}\frac{(-1)^{i+j}}{(x_i - x_j)}, \qquad i \neq j, \quad i,j = 0, \ldots, N,$$

where

$$c_i = \begin{cases} 2, & i = 0 \text{ or } N, \\ 1, & \text{otherwise.} \end{cases}$$

Graphically,



Matlab code for this matrix is given in Trefethen's text and available for download at the author's website.

Remarkably, the m-th derivative matrix coincides with D^m (STW Thm. 3.10). Of course, it is inefficient to use D^m ($\mathcal{O}(N^3)$ operations.) Improved formulae run at $\mathcal{O}(N^2)$ cost (Trefethen p. 61 cites Gottlieb and Lustman (1983).) For the simple examples we will consider, such additional efficiency is not necessary.

For values of N larger than a threshold (e.g. $N \geq 32$, or $N \geq 64$, etc., depending on the computer, the compiler, etc.) it is more efficient to perform the differentiations by means of FFT.

FFT-based Chebyshev differentiation

(backward recurrence)

$$v(x) = (I_N u)(x) = \sum_{n=0}^{N} \tilde{u}_n T_n(x)$$

In view of the relation

$$2T_n(x) = \frac{1}{n+1} T'_{n+1}(x) - \frac{1}{n-1} T'_{n-1}(x),$$

which follows easily from

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

we obtain

$$v'(x) = \sum_{n=1}^{N} \tilde{u}_n T'_n(x) =$$

$\tilde{\mu}^{(1)}_N = 0$

$$= \sum_{n=0}^{N} \tilde{\mu}^{(1)}_n T_n(x) =$$

$$= \tilde{\mu}^{(1)}_0 \underbrace{1}_{T_1'} + \tilde{\mu}^{(1)}_1 \underbrace{T_1}_{\frac{1}{4}T_2'} +$$

$$+ \sum_{n=2}^{N-1} \tilde{\mu}^{(1)}_n \left(\frac{T'_{n+1}}{2(n+1)} - \frac{T'_{n-1}}{2(n-1)} \right)$$

Therefore, by orthogonality of the polynomials $T_n'(x)$ with respect to the weight $(1-x^2)^{1/2}$, we have

$$\tilde{\mu}^{(1)}_N = 0,$$

$$\text{Coeff. of } T_1' : \quad \tilde{\mu}_1 = \tilde{\mu}^{(1)}_0 - \frac{\tilde{\mu}^{(1)}_2}{2}$$

$$\Longrightarrow \quad \tilde{\mu}^{(1)}_0 = \left(2\tilde{\mu}_1 + \tilde{\mu}^{(1)}_2\right)/2$$

Orthogonality: Above and in what follows we use that the derivatives of the Chebyshev polynomials are orthogonal with respect to the weight $(1-x^2)^{1/2}$. This follows from the Sturm-Liouville equation we obtained last class for the Chebyshev polynomials:

$$\frac{d}{dx}\left[\sqrt{1-x^2}\left(\frac{dT_k}{dx}\right)\right] + k^2 \frac{1}{\sqrt{1-x^2}} T_k = 0$$

Coeff of T_n', $n=4,\dots,N-2$.

$$\tilde{u}_n = \frac{\tilde{u}^{(1)}_{n-1}}{2n} - \frac{\tilde{u}^{(1)}_{n+1}}{2n}$$

$$\Longrightarrow \quad \tilde{u}^{(1)}_{n-1} = 2n\,\tilde{u}_n + \tilde{u}^{(1)}_{n+1} \qquad n=4,\dots,N-2$$

Thus,

$$\tilde{u}^{(1)}_N = 0$$

$$\tilde{u}^{(1)}_0 = \left(2\tilde{u}_1 + \tilde{u}^{(1)}_2\right)/2$$

$$\tilde{u}^{(1)}_1 = 4\tilde{u}_2 + \tilde{u}^{(1)}_3$$

$$\vdots$$

In sum $\quad \tilde{u}^{(1)}_N = 0$

$$\tilde{u}^{(1)}_{N-1} = 2N\,\tilde{u}_N$$

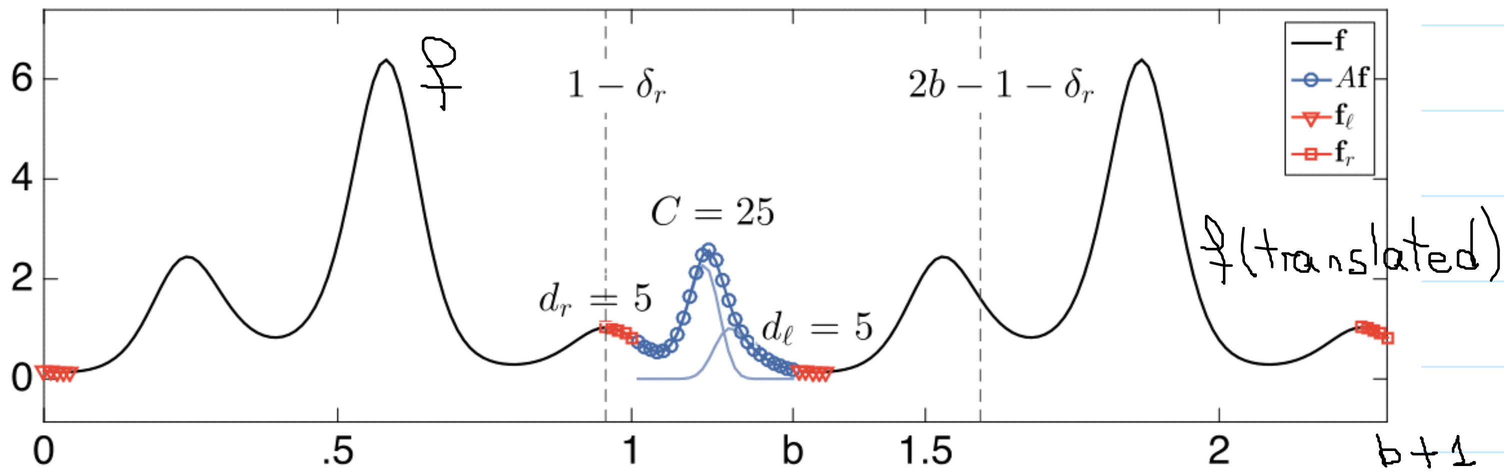
$$\tilde{u}^{(1)}_{n-1} = \left(2n\,\tilde{u}_n + \tilde{u}^{(1)}_{n+1}\right)/c_{n-1}$$

$(n = N-1, \dots, 1)$

$(c_0 = 2,\ c_n = 1 \text{ for } n \geq 1)$

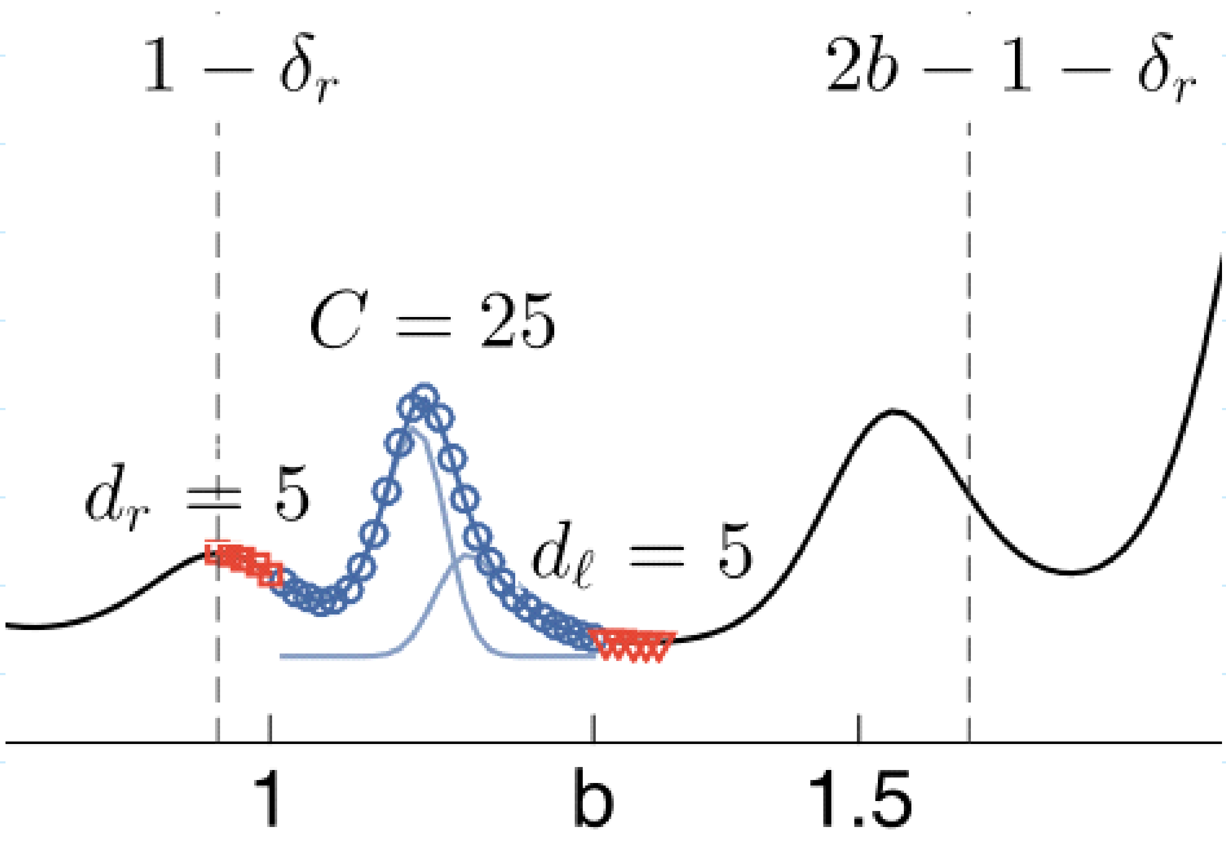
Fourier Continuation

(Brief presentation, see e.g Journal of Computational Physics 307 (2016) pp. 333–354, Amlani + Bruno.)



Idea: utilize a linear algebra calculation to obtain continuation values onto a translation of the given function $f : [0,1] \longrightarrow \mathbb{R}$

In more detail, using e.g. $d = 5$ points, blend the curve to zero towards left and right. Then add the results.



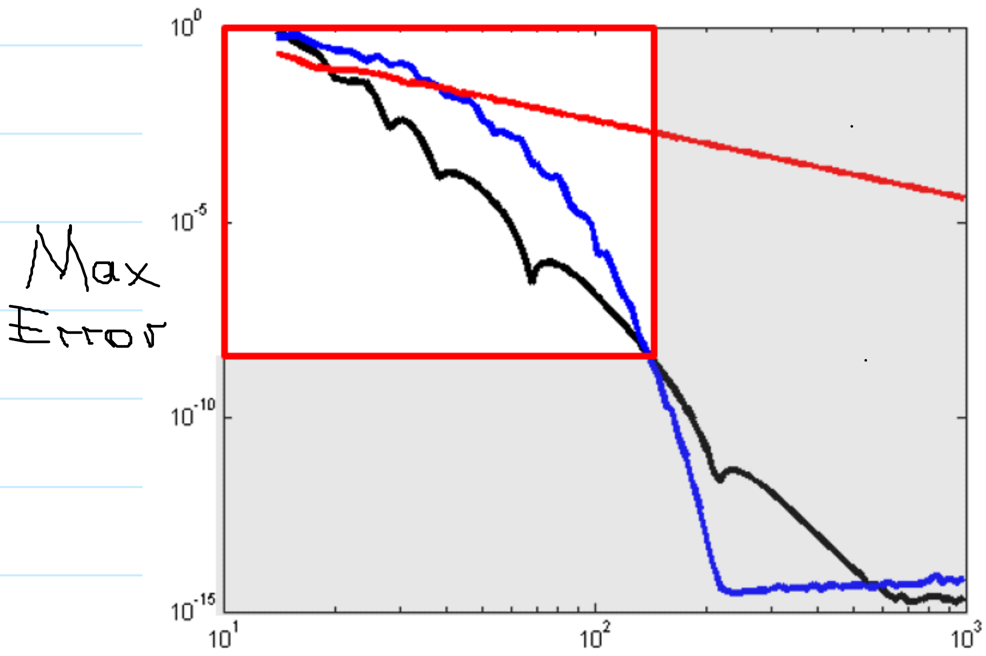
Let us consider the rightward extension to zero.

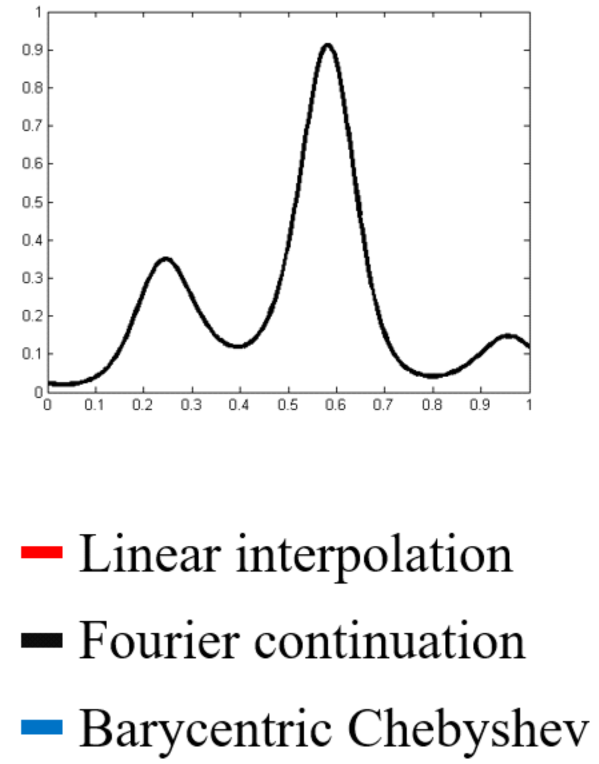
A $\underbrace{\text{Fourier expansion}}_{\text{auxiliary}}$ is sought, with periodicity interval $[1-\delta_r, 2b-1-\delta_r]$ which matches the given point values for a small number of points (e.g. $d_r = 5$ points), and which is equal to zero for a number d_ℓ of points (e.g. $d_\ell = 5$)

to the right of b.

This is accomplished by using a polynomial interpolant for the d_r given function values, and then oversampling the polynomial and the zero values, and determining the Fourier coefficients by means of a least-squares procedure. The auxiliary Fourier expansion is used to obtain a number C (e.g. 25) of continuation values. This thus provides discrete values of a periodic function, the Fourier continuation, whose Fourier coefficients can be obtained via FFT.

Example: Order-10 Fourier Continuation of the function considered above





FC does not cluster points towards endpoints!

Significant effect on smallness of step size required for stability.