4.4 Collocation based on trigonometric interpolation

Consider 1D-Schrödinger equation on the real line. Since the L^2-function ψ can be assumed to be negligible outside an interval $[-T, T]$, we consider without restriction of generality

$$i\dot{\psi}(x,t) = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2}(x,t) + V(x)\psi(x,t), \quad x \in [-\pi, \pi],$$

$$\psi(-\pi, t) = \psi(\pi, t) \quad \forall t.$$

Trigonometric Interpolation:

$$\psi \approx \psi_K = \sum_{k=-\frac{K}{2}}^{K/2-1} c_k(t) e^{ikx}, \qquad x \in [-\pi, \pi], \; K \text{ even}$$

In this case, instead of a Galerkin method, we consider collocation on an equidistant grid

$x_j = j \cdot \frac{2\pi}{K}$, $j = -\frac{K}{2}, \dots, \frac{K}{2} - 1$, thus requiring

$$i\dot{\psi}_K(x_j, t) = -\frac{1}{2}\frac{\partial^2\psi_K}{\partial x^2}(x_j, t) + V(x_j)\psi_k(x_j, t), \; j = -\frac{K}{2}, \dots, \frac{K}{2} - 1.$$

Discrete Fourier Transform

Let $\mathcal{F}_K : \mathbb{C}^K \to \mathbb{C}^K$ denote the Discrete Fourier Transform of length K,

$$\hat{v} = \mathcal{F}_K v \quad \text{with } \hat{v}_k = \frac{1}{K} \sum_{j=-\frac{K}{2}}^{\frac{K}{2}-1} e^{-ikj\,2\pi/K} v_j \,, \; k = -\frac{K}{2}, \dots, \frac{K}{2}-1$$

The inverse transform $\mathcal{F}_K^{-1}$ is given by

$$v = \mathcal{F}_K^{-1} \hat{v} \quad \text{with } v_j = \sum_{k=-\frac{K}{2}}^{\frac{K}{2}-1} e^{ijk\,2\pi/K} \hat{v}_k \,, \; j = -\frac{K}{2}, \dots, \frac{K}{2}-1.$$

The two transforms can be implemented with computational complexity $O(K \log K)$ via the Fast Fourier Transform (FFT) see [41, 42, 43].

Define $D_K := \frac{1}{2} \operatorname{diag}(k^2)_{k=-\frac{K}{2}}^{\frac{K}{2}-1}$, $V_K := \operatorname{diag}(V(x_j))_{j=-\frac{K}{2}}^{\frac{K}{2}-1}$

Noting $\psi_K(x_j, t) = \mathcal{F}_K^{-1}(c_k(t))$, we obtain

$$i\dot{c} = D_K c + \mathcal{F}_K V_K \mathcal{F}_K^{-1} c,$$

or alternatively for $u_j(t) = \psi_K(x_j, t)$

$$i\dot{u} = \mathcal{F}_K^{-1} D_K \mathcal{F}_K u + V_K u.$$

Trigonometric Interpolation by FFT (Fast Fourier Transform)

<u>Theorem</u>: The trigonometric polynomial $p(x) = \sum_{j=0}^{N-1} \beta_j e^{jix}$ satisfies $p(x_k) = f_k$, $k = 0, 1, \dots, N-1$ for $x_k = \frac{2k\pi}{N}$ iff

$$\beta_j = \frac{1}{N} \sum_{k=0}^{N-1} f_k e^{-2\pi i j k/N}, \quad j = 0, \dots, N-1.$$

<u>Proof</u>: [43]

<u>FFT</u> (Cooley/Tukey 1965 [41])

Let $N = 2^n$ (for simplicity). Define $q(x), r(x)$ of order $M := \frac{N}{2}$:

$$q(x_{2k}) = f_{2k}, \quad r(x_{2k}) = f_{2k+1}, \quad k = 0, \dots, M-1$$

$$e^{iMx_k} = \begin{cases} 1, & k \text{ even} \\ -1, & k \text{ odd} \end{cases}$$

$$\Rightarrow \tilde{p}(x) := q(x)\left(\frac{1+e^{iMx}}{2}\right) + r\left(x - \frac{\pi}{M}\right)\left(\frac{1-e^{iMx}}{2}\right)$$

interpolates x_k, $k = 0, \dots, N-1$, order $\tilde{p} = 2M = N \Rightarrow \tilde{p} \equiv p$.

<u>m-th step of FFT</u>: Determine R trigonometric polynomials

$$p_r^{(m)}(x) = \beta_{r,0}^{(m)} + \dots + \beta_{r,2M-1}^{(m)} e^{i(2M-1)x}, \quad r = 0, \dots, R-1 \text{ by}$$

$$2p_r^{(m)}(x) = p_r^{(m-1)}(x)\left(1 + e^{iMx}\right) + p_{R+r}^{(m-1)}\left(x - \frac{\pi}{M}\right)\left(1 - e^{iMx}\right) \Leftrightarrow$$

$$2\beta_{r,j}^{(m)} = \beta_{r,j}^{(m-1)} + \beta_{R+r,j}^{(m-1)} \varepsilon_m^j$$

$$2\beta_{r,M+j}^{(m)} = \beta_{r,j}^{(m-1)} - \beta_{R+r,j}^{(m-1)} \varepsilon_m^j$$

$$\varepsilon_m = \exp(-\pi i/M)$$

$$r = 0, \dots, R-1, \quad j = 0, \dots, M-1.$$

Computational complexity: $\sim N \log(N)$

Approximation Properties:

Denote the trigonometric interpolation operator by I_K,

$$I_K f(x) = \sum_{k=-\frac{K}{2}}^{\frac{K}{2}-1} c_k e^{ikx} \quad \text{with} \quad (c_k) = \tilde{F}_K(f(x_j)).$$

Theorem: Suppose that f is a 2π-periodic function for which the s-th derivative $\partial_x^s f \in L^2$ for some $s \geq 1$. Then, the interpolation error is bounded by

$$\| f - I_K f \|_{L^2} \leq C K^{-s} \| \partial_x^s f \|,$$

where C depends only on s.

Proof: Write

$$f(x) = \sum_{k=-\infty}^{\infty} a_k e^{ikx}, \quad I_K f(x) = \sum_{k=-\frac{K}{2}}^{\frac{K}{2}-1} c_k e^{ikx},$$

$$c_k = \sum_{e=-\infty}^{\infty} a_{k+eK} \quad (\text{"aliasing formula"}).$$

Using Parseval's formula,

For $$f(x) = \sum_{k=-\infty}^{\infty} b_k e^{ikx}, \quad \|f\|_{L^2}^2 = \sum_{k=-\infty}^{\infty} |b_k|^2$$

and the Cauchy-Schwarz inequality,

$$\left| \sum_{k=-\infty}^{\infty} a_k b_k \right| \leq \sqrt{\sum_{k=-\infty}^{\infty} |a_k|^2} \sqrt{\sum_{k=-\infty}^{\infty} |b_k|^2}$$

we find

$$\|f - I_K f\|^2 = \sum_{k=-\frac{K}{2}}^{\frac{K}{2}-1} \Big| a_k - \sum_{\ell=-\infty}^{\infty} a_{k+\ell K} \Big|^2 + \sum_{k \in \mathbb{Z} \setminus \{-\frac{K}{2}, \dots, \frac{K}{2}-1\}} |a_k|^2 =$$

$$= \sum_{k=-\frac{K}{2}}^{\frac{K}{2}-1} \left(\Big| \sum_{\ell \neq 0} a_{k+\ell K} \Big|^2 + \sum_{\ell \neq 0} |a_{k+\ell K}|^2 \right) \leq$$

$$\leq \sum_{k=-\frac{K}{2}}^{\frac{K}{2}-1} \Big(\sum_{\ell \neq 0} (k+\ell K)^{-2s} \sum_{\ell \neq 0} (k+\ell K)^{2s} |a_{k+\ell K}|^2 +$$

$$+ \sum_{\ell \neq 0} (k+\ell K)^{-2s} (k+\ell K)^{2s} |a_{k+\ell K}|^2 \Big) \leq$$

$$\leq C^2 K^{-2s} \sum_{k=-\infty}^{\infty} |k^s a_k|^2 = C^2 K^{-2s} \|\partial_x^s f\|^2.$$

Here, we used

$$\partial_x^s f = \sum_{k=-\infty}^{\infty} k^s a_k e^{ikx}$$

for $f = \sum_{k=-\infty}^{\infty} a_k e^{ikx}$.

<u>Theorem</u>: Suppose the exact solution has $\partial_x^{s+2} \psi(\cdot, t) \in L^2$, for some $s \geq 1$. Then the error of Fourier collocation with initial value $\psi_K(x,0) = I_K \psi(x,0)$ satisfies

$$\|\psi_K(t) - \psi(t)\|_{L^2} \leq C K^{-s} (1+t) \max_{0 \leq \tau \leq t} \|\partial_x^{s+2} \psi(\tau)\|,$$

where C depends only on s.

<u>Proof</u>: [14].