Introduction to spectral methods in Matlab II

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Introduction

- numerical solution of a PDE: approximate solution with finite precision on a numerical grid (discretization)
- methods:
    - finite differences (1950s): local polynomials of low order
    - finite elements (1960s): local smooth functions
    - spectral methods (1970s): global smooth functions

Differentiation matrices

- function $u(x)$ given on a number of grid points, $\{x_i\}$, $u(x_i) = u_i$, $i = 0, 1, \ldots, N$. Approximation w_i of the derivative of u at the grid points?
- Consider uniform grid $x_{i+i} - x_i = h$, $i = 0, 1, \ldots, N-1$ and periodic boundary conditions $u_{i+N} = u_i \; \forall i$.
- symmetric, second order approximation of the derivative:

$$w_j = \frac{u_{j+1} - u_{j-1}}{2h}$$

vector notation:

$$\vec{w} = D_N \vec{u}$$

- differentiation matrix

$$D_N = \frac{1}{2h} \begin{pmatrix} 0 & 1 & & & -1 \\ -1 & 0 & \ddots & & \\ & -1 & \ddots & & \\ & & \ddots & 0 & 1 \\ 1 & & & -1 & 0 \end{pmatrix}$$

Toeplitz matrix (built from two vectors) and circulant (built from one vector)

- alternative way: local interpolation of u and differentiation of the interpolation polynomial: Let p_j be the unique polynomial of degree ≤ 2 with $p_j(x_{j-1}) = u_{j-1}$, $p_j(x_{j+1}) = u_{j+1}$ and $p_j(x_j) = u_j \ \forall j$.

- Lagrange polynomial

$$p_j(x) = \frac{(x-x_j)(x-x_{j+1})}{2h^2} u_{j-1} - \frac{(x-x_{j+1})(x-x_{j-1})}{h^2} u_j + \frac{(x-x_j)(x-x_{j-1})}{2h^2} u_{j+1}$$

- $w_j = p'(x_j) = \frac{1}{2h}(u_{j+1} - u_j)$

- generalization to higher orders. Fourth order: unique interpolation polynomial with $p_j(x_{j\pm 2}) = u_{j\pm 2}$, $p_j(x_{j\pm 1}) = u_{j\pm 1}$, $p_j(x_j) = u_j$. Put $w_j = p_j'(x_j)$.

- differentiation matrix

$$D_N = \frac{1}{h} \begin{pmatrix} & & \ddots & & & \frac{1}{12} & -\frac{2}{3} \\ & & \ddots & -\frac{1}{12} & & & \frac{1}{12} \\ & & \ddots & \frac{2}{3} & \ddots & & \\ & & \ddots & 0 & \ddots & & \\ & & \ddots & \frac{2}{3} & \ddots & & \\ -\frac{1}{12} & & & \frac{1}{12} & \ddots & & \\ \frac{2}{3} & -\frac{1}{12} & & & \ddots & & \end{pmatrix}$$

- Example: $u(x) = e^{\sin x}$, $x \in [-\pi, \pi]$; compare numerical solution with $u'(x) = \cos x e^{\sin x}$ for various N: 4th order convergence.

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- spectral method: interpolation polynomial on the whole grid via a single function $p(x)$. Periodic problem: trigonometric polynomial (truncated Fourier series). Non-periodic domains: orthogonal polynomials on non-uniform grids (here Chebyshev)

- periodic case, N even

$$D_N = \frac{1}{2}\begin{pmatrix} \ddots & \vdots & \\ \ddots & -\cot(2h/2) & \\ \ddots & \cot(h/2) & \ddots \\ \ddots & 0 & \ddots \\ \ddots & -\cot(h/2) & \ddots \\ & \cot(2h/2) & \ddots \\ & \vdots & \ddots \end{pmatrix}$$

Toeplitz and circulant

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- convergence:
finite difference: $0(N^{-m})$
spectral method for C^∞ function: $0(N^{-m})\ \forall m$ (exponential convergence, 'spectral accuracy')

Fourier series

- action of a circulant matrix:
  $w_i = \sum_{j=0}^{N} D_{ij} v_j = \sum_{j=0}^{N} D(i-j) v_j$: convolution. Convolutions in physical space become products in Fourier space. Thus it is convenient to consider Fourier transforms.

- periodic function $f(x)$, $f(x+2k\Box) = f(x)$, $k \in \mathbb{Z}$:

$$f(x) = \sum_{k\in\mathbb{Z}} \hat{f}(k) e^{-ikx}, \quad \hat{f}(k) = \frac{1}{2\Box} \int_{-\pi}^{\pi} f(x) e^{ikx} dx$$

$(f(x) \in \mathrm{L}^2([-\Box, \Box]),\ \hat{f} \in l^2(\mathbb{Z}))$

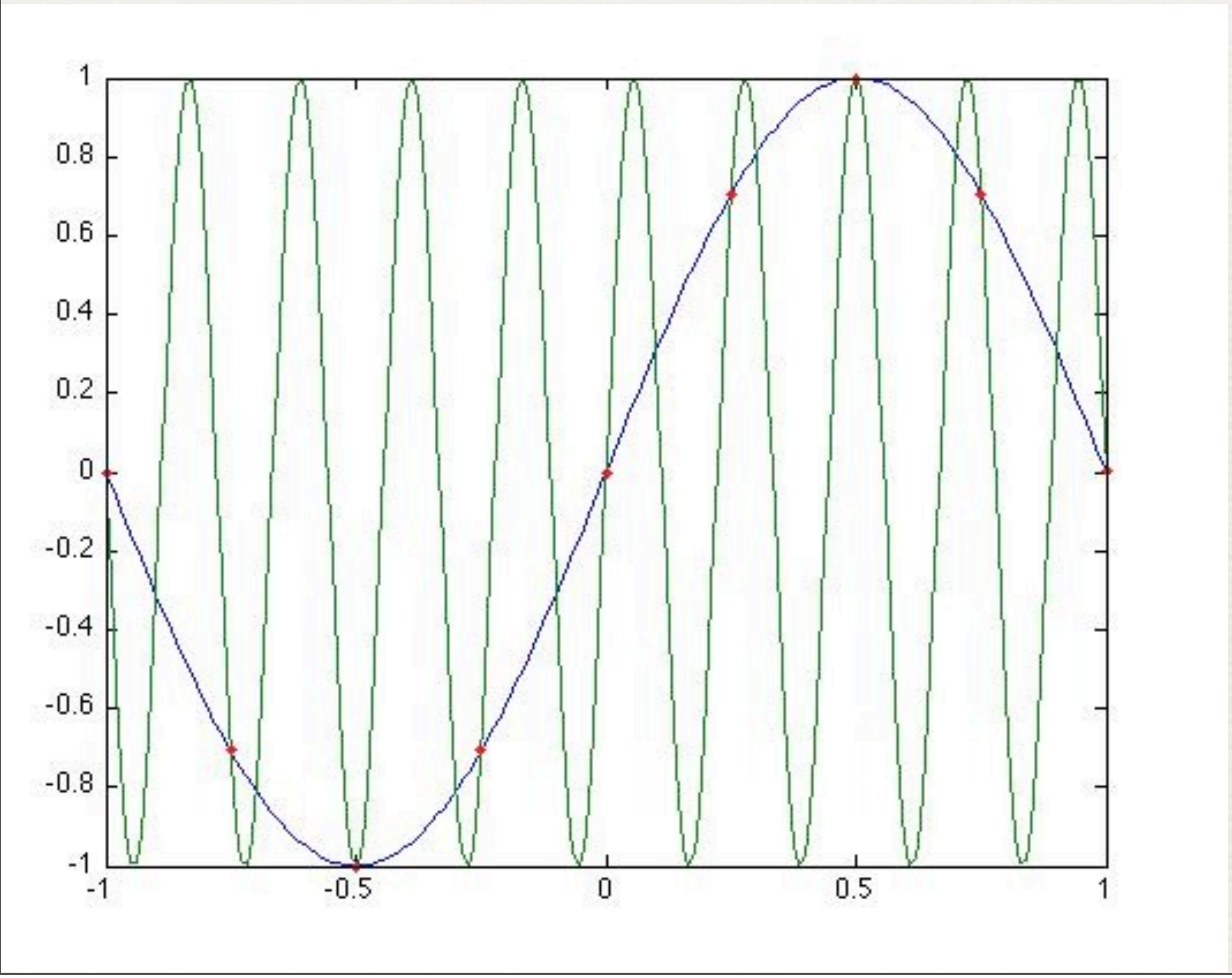
- formal exchange $k \leftrightarrow x$, rescaling with h, no periodicity in x:
  $x \in h\mathbb{Z}$, $v(x_j) = v_j$, $j \in \mathbb{Z}$,

$$\hat{v}(k) = h \sum_{j=-\infty}^{\infty} e^{-ikx_j} v_j, \quad v_j = \frac{1}{2\Box} \int_{\pi/h}^{\pi/h} e^{ikx_j} \hat{v}(k) dk$$

$k \in [-\Box/h, \Box/h]$.

Aliasing

- $e^{ik_1 x} = e^{ik_2 x}$ implies $k_1 = k_2$ for $x \in \mathbb{R}$, but only $k_1 - k_2 = \frac{2\pi}{h} n$, $n \in \mathbb{Z}$, for $x \in h\mathbb{Z}$; the additional values for $n \neq 0$ are called ‘aliases’ of k.



$\sin(\pi x)$ and $\sin(9\pi x)$ equivalent on the grid $\frac{1}{4}\mathbb{Z}$

Spectral differentiation

- interpolant for spectral differentiation:

$$p(x) = \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} e^{ikx}\hat{v}(k)dk, \quad x \in \mathbb{R}$$

  $p(x)$ analytic, $p(x_j) = v_j \ \forall j$.
  Fourier transform:

$$\hat{p}(k) = \begin{cases} \hat{v}(k) & k \in [-\pi/h, \pi/h] \\ 0 & \text{otherwise} \end{cases}$$

  compact support, band-limited interpolant of v (unique for band $[-\pi/h, \pi/h]$), *sampling theorem.*

- spectral derivative: $w_j = p'(x_j)$ via $\widehat{v'}(k) = ik\hat{v}(k)$. In words:
  - given v, compute $\hat{v}(k)$
  - define $\hat{w} = ik\hat{v}(k)$
  - compute w

- computation of the differentiation matrix via convolution with the Kronecker δ as function v,

$$\delta_j = \begin{cases} 1 & j = 0 \\ 0 & j \neq 0 \end{cases} \qquad \hat{\delta} = h$$

interpolant:

$$p(x) = \frac{h}{2\pi} \int_{-\pi/h}^{\pi/h} e^{ikx} dk = \operatorname{sinc} \frac{\pi x}{h} =: S_h(x)$$

$\operatorname{sinc}(\mathrm{x}) = \frac{\sin x}{x}$.

- general function v (convolution with δ): $v_j = \sum_{m=-\infty}^{\infty} v_m \delta_{j-m}$. Thus

$$p(x) = \sum_{-\infty}^{\infty} v_m S_h(x - x_m)$$

and $w_j = p'(x_j) = \sum_{m \in \mathbb{Z}} v_m S_h'(x_j - x_m)$, infinite matrix

$$S_h'(x_j) = \begin{cases} 0 & j = 0 \\ \frac{(-1)^j}{jh} & j \neq 0 \end{cases}$$

Spectral differentiation via FT

- periodic function: $v_{j+mN} = v_j$, $j, m \in \mathbb{Z}$; spacing $h = \frac{2\pi}{N}$, choose N even. In this case the wave numbers k, $k \in [-\pi/h, \pi/h]$, are also discrete since e^{ikx} only periodic for integer wave numbers: discrete Fourier transform (DFT)

$$\hat{v}_k = h \sum_{j=1}^{N} e^{-ikx_j} v_j, \quad k = -\frac{N}{2}+1, \ldots, \frac{N}{2},$$

$$v_j = \frac{1}{2\pi} \sum_{k=-N/2+1}^{N/2} e^{\,ikx_j} \hat{v}_k, \quad j = 1, \ldots, N$$

for spectral differentiation symmetrization useful:

$$v_j = \frac{1}{2\pi} \sum_{k=-N/2+1}^{N/2-1} e^{\,ikx_j} \hat{v}_k + \frac{1}{4\pi} \left(\hat{v}_{-N/2} e^{-ix_j N/2} + \hat{v}_{N/2} e^{ix_j N/2} \right), \quad j = 1, \ldots, N$$

- band limited interpolant $p(x) = v(x)$, trigonometric polynomial of degree $\leq N/2$; interpolant of translated periodic δ-function

$$\delta_j = \begin{cases} 1 & j = 0 \pmod N \\ 0 & j \neq 0 \pmod N \end{cases}$$

Fourier transform $\hat{\delta}_k = h \ \forall k$. This implies for the interpolant

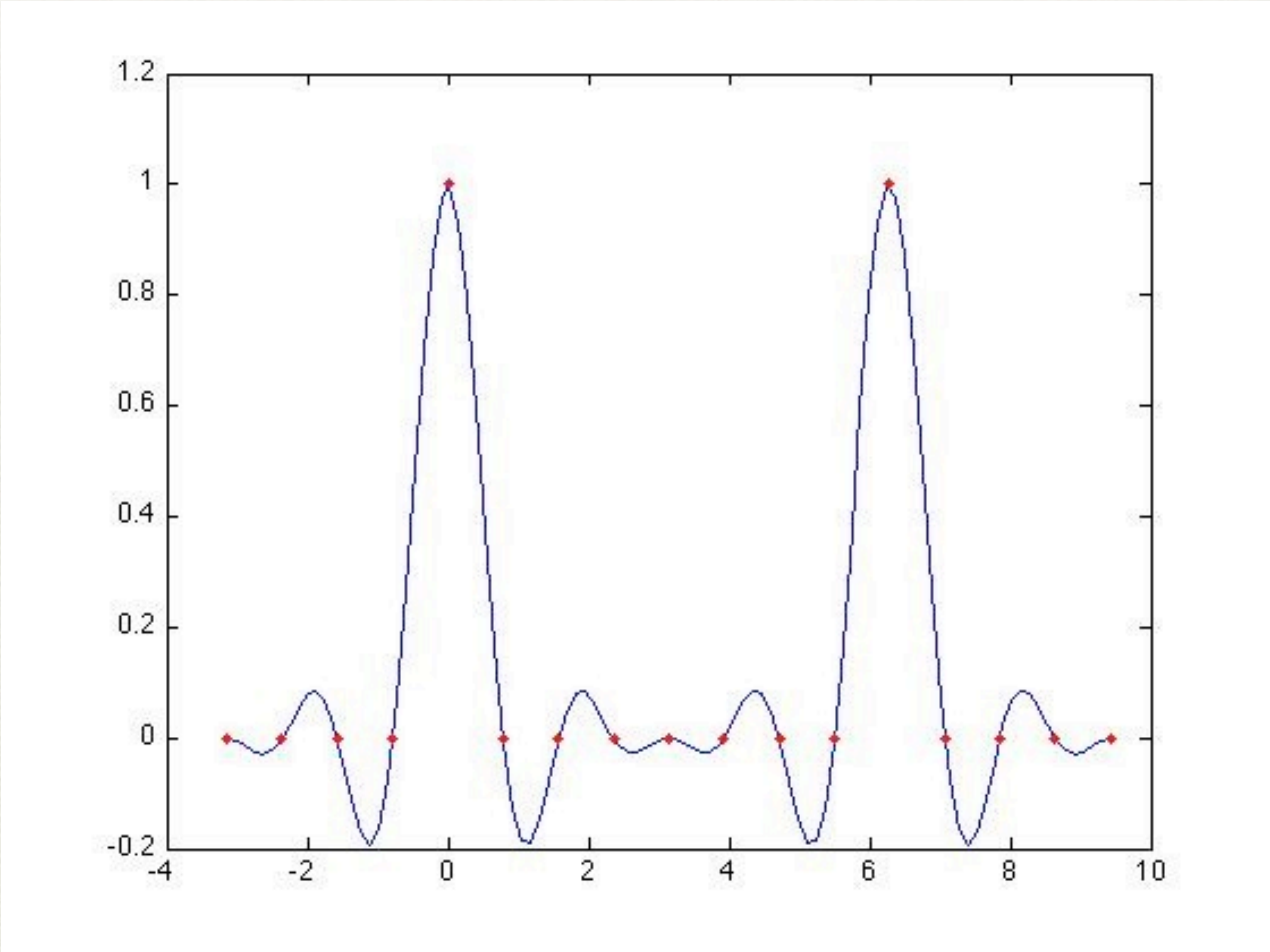
$$\begin{aligned} p(x) &= \frac{h}{2\pi} \left(\frac{1}{2} \sum_{k=-N/2}^{N/2-1} e^{ikx} + \frac{1}{2} \sum_{k=-N/2+1}^{N/2} e^{ikx} \right) \\ &= \frac{h}{2\pi} \cos\frac{x}{2} \frac{\sin(Nx/2)}{\sin(x/2)} =: S_N \end{aligned}$$

periodic sinc function

$$S_N'(x_j) = \begin{cases} 0 & j = 0 \pmod N \\ \frac{1}{2}(-1)^j \cot \frac{jh}{2} & j \neq 0 \pmod N \end{cases}$$

gives the differentiation matrix.

Periodic *sinc*-function



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Periodicity and DFT

- equivalent approach via DFT:
  - given v, compute $\hat{v}$
  - define $\hat{w}_k = ik\hat{v}_k$ ($\hat{w}_{N/2} = 0$)
  - compute w
- fast Fourier transform (FFT), 1965 by Cooley and Tuckey, 1805 by Gauss: if N is a product of primes, $O(N \log N)$ floating point operations. Matlab: wave vector $0, 1, \ldots, N/2, -N/2+1, -N/2+2, \ldots, -1$; works on complex vector (factor 2 lost for real vectors).

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Smoothness and spectral accuracy

- convergence of Fourier series (Dirichlet): if u is piecewise continuous, then $\sum_{k\in\mathbb{Z}} \hat{u}(k)e^{ikx}$ converges to u. Consequently if $u \in C^m$, the Fourier series converges for $u^{(m-1)}$, i.e., $\sum_{k\in\mathbb{Z}} k^{m-1}\hat{u}(k)e^{ikx}$. The smoother a function in physical space, the more it is localized in Fourier space.

- **theorem 1** *Smoothness of a function and decay of its Fourier transform* *Let* $u \in \mathrm{L}^2(\mathbb{R})$ *have Fourier transform* $\hat{u}(k)$.

  1. *If* $u \in C^{p-1}(\mathbb{R})$ *for some* $p \geq 0$ *and has a pth derivative of bounded variation, then*

  $$\hat{u}(k) = O(|k|^{-p-1}) \text{ as } |k| \to \infty \ .$$

  2. *If* $u \in C^{\infty}(\mathbb{R})$, *then*

  $$\hat{u}(k) = O(|k|^{-m}) \text{ as } |k| \to \infty$$

  for every $m \geq 0$. *The converse also holds.*

  3. *If there exist* $a, c > 0$ *such that* u *can be extended to an analytic function in the complex strip* $|\Im z| < a$ *with* $||u(\cdot + iy)||$ *uniformly for all* $y \in [-a, a]$, *where* $||u(\cdot + iy)||$ *is the* L^2 *norm along the horizontal line* $\Im z = y$, *then* $u_a \in L^2(\mathbb{R})$, *where* $u_a(k) = e^{a|k|}\hat{u}(k)$. *The converse also holds.*

  4. *If* u *can be extended to an entire function (i.e., analytic throughout the complex plane) and there exists* $a > 0$ *such that* $|u(z)| = o(e^{a|z|})$ *as* $|z| \to \infty$ $\forall z \in \mathbb{C}$, *then* $\hat{u}$ *has compact support in* $[-a, a]$.

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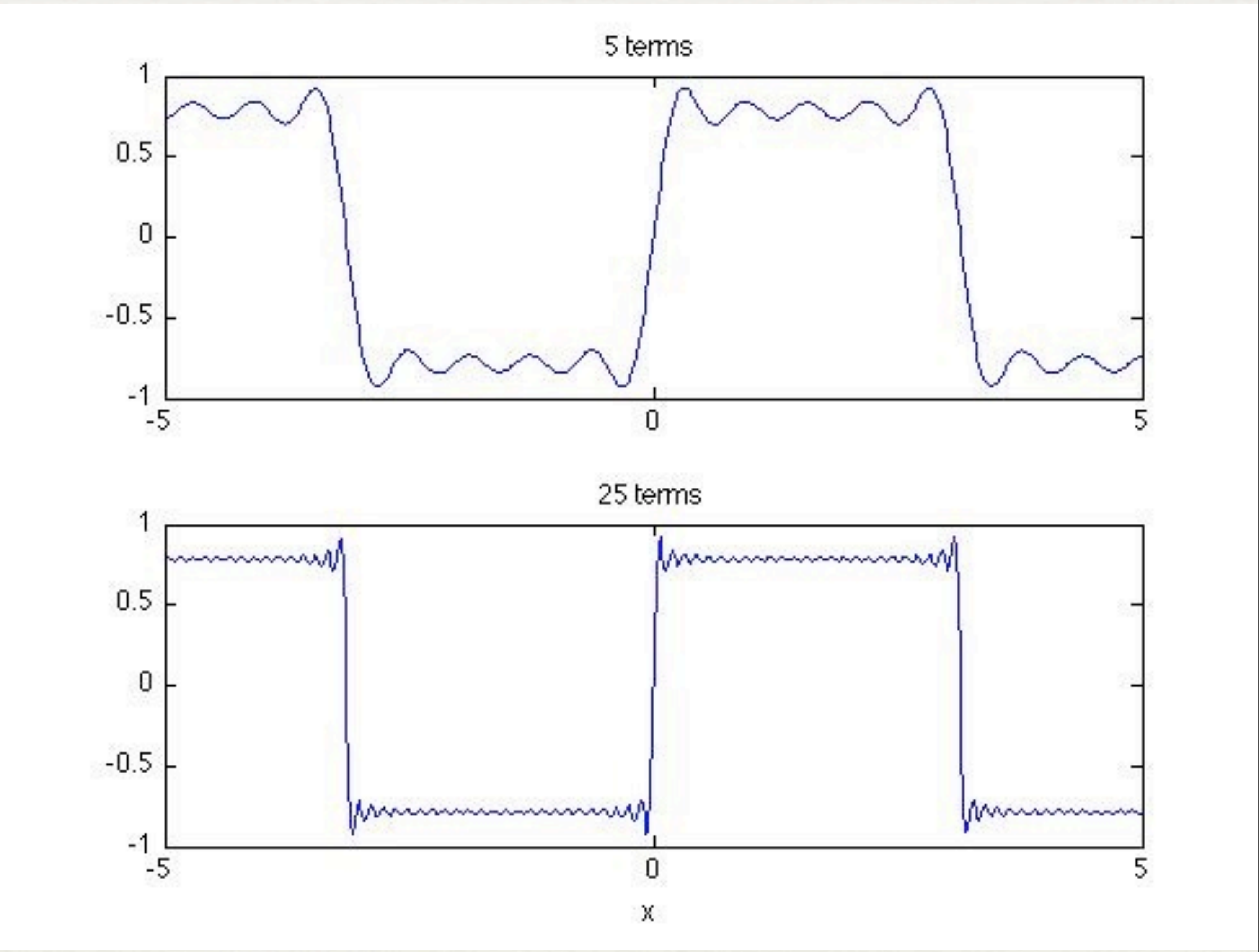
Gibbs phenomenon

- convergence of Fourier series at discontinuities of the the function: strong oscillations, `overshooting‘ by roughly 9%
- the Fourier series for the step function (5 respectively 25 terms)



- **theorem 2** *Aliasing formula*
  Let $u \in L^2(\mathbb{R})$ have a first derivative with bounded variation, and let v be the grid function on $h\mathbb{Z}$ defined by $v_j = u(x_j)$. Then $\forall k \in [-\pi/h, \pi/h]$,

$$\hat{v}(k) = \sum_{j \in \mathbb{Z}} \hat{u}(k + 2\pi j/h)$$

  This implies that

$$\hat{v}(k) - \hat{u}(k) = \sum_{j \in \mathbb{Z}, j \neq 0} \hat{u}(k + 2\pi j/h).$$

  Smoothness can be related to the error $\hat{v}(k) - \hat{u}(k)$ (*aliasing error*).

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