Numerical Methods
in Engineering and Applied Science

Lecture 15. Spectral methods.

Let us consider a semi-discrete transform,

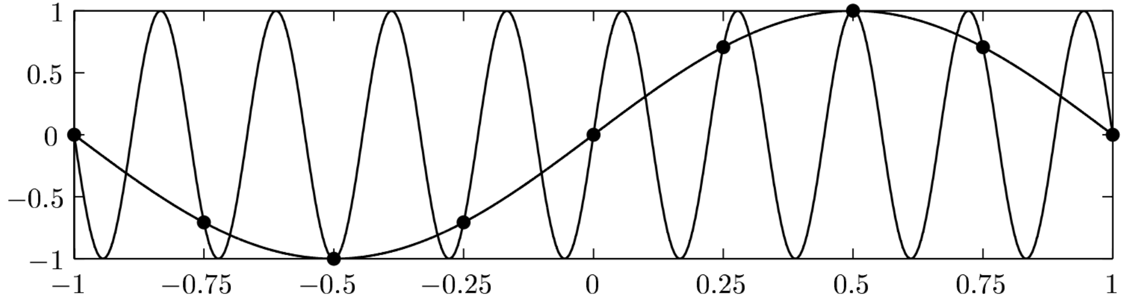
$$\hat{v}(k) = h \sum_{j=-\infty}^{\infty} e^{-ikx_j} v_j, \quad k \in [-\pi/h, \pi/h],$$

$$v_j = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{ikx_j} \hat{v}(k) dk, \quad j \in \mathbb{Z}.$$

$$\begin{array}{lcllcl} \text{Physical domain} & : & \text{discrete,} & \text{unbounded} & : & x \in h\mathbb{Z} \\ & & \updownarrow & \updownarrow & & \\ \text{Spectral domain} & : & \text{bounded,} & \text{continuous} & : & k \in [-\pi/h, \pi/h] \end{array}$$

Aliasing. Consider two functions, $f(x) = \exp(ik_1x)$ et $g(x) = \exp(ik_2x)$. These functions cannot be identical everywhere on $\mathbb{R}$ if $k_1 \neq k_2$. On the other hand, if $k_1 - k_2$ is an integer multiple of $2\pi/h$, the values $f_j = \exp(ik_1x_j)$ and $g_j = \exp(ik_2x_j)$ can be equal, $f_j = g_j$ for all j.

It suffices to define the wavenumbers on the interval of length $2\pi/h$. We choose the interval $[-\pi/h, \pi/h]$.



To obtain a numerical method for calculating the derivative, we define the interpolating function

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

It is an analytic function of x, with $p(x_j) = v_j$ for all j. By construction, $\hat{p}(k)$ is compactly supported on $k \in [-\pi/h, \pi/h]$.

For a function v defined on $h\mathbb{Z}$, there is only one interpolating function (1). We obtain a numerical method for calculating the derivative:

- Given v, determine the function p (1).
- $w_j = p'(x_j)$.

We can rewrite this algorithm:

- Given v, compute the semi-discrete Fourier transform $\hat{v}$.
- Calculate $\hat{w}(k) = ik\hat{v}(k)$.
- Calculate w from $\hat{w}$ by the inverse transform.

We recall that, for the Fourier transform of a derivable function $\hat{u}$,

$$\widehat{u'}(k) = ik\hat{u}(k).$$

Consider the function

$$\delta_j = \begin{cases} 1 & j = 0, \\ 0 & j \neq 0. \end{cases}$$

The Fourier transform of this function is a constant, $\hat{\delta} = h$ for all $k \in [-\pi/h, \pi/h]$. We see that the interpolating function of δ is

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

with $p = 1$ at $x = 0$. We will use the notation

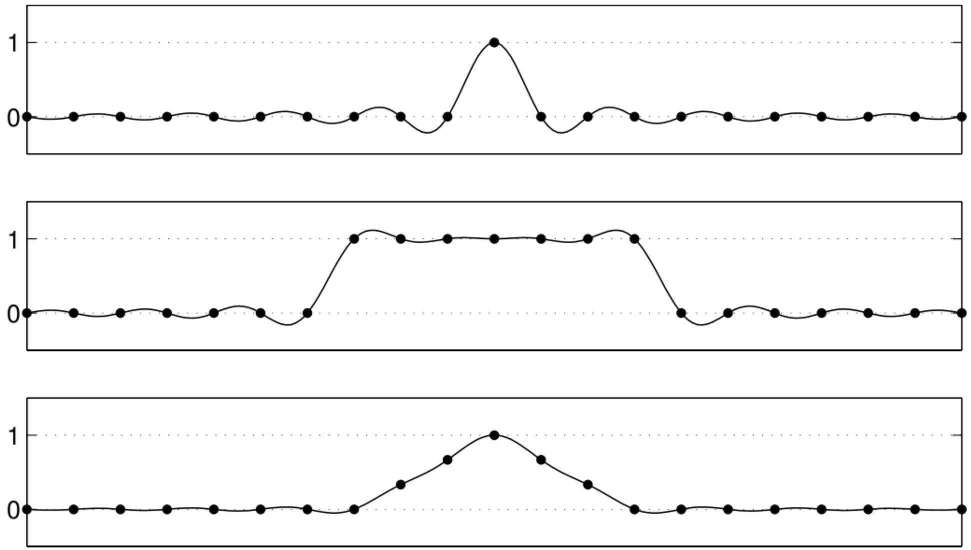
$$S_h = \operatorname{sinc}(x/h).$$

Note that the interpolating function of δ_{j-m} is $S_h(x - x_m)$. For any function v on $\{x_j\}$,

$$v_j = \sum_{m=-\infty}^{\infty} v_m \delta_{j-m}.$$

Since the Fourier transform is linear, we get

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



The derivative is equal to

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

We can rewrite it in the form

$$w = Dv \quad \text{avec} \quad D_{ij} = \begin{cases} 0 & i = j, \\ \dfrac{(-1)^{(i-j)}}{(i-j)h} & i \neq j. \end{cases}$$

$$D = \frac{1}{h} \begin{pmatrix} & \vdots & \\ \ddots & \frac{1}{3} & \\ \ddots & -\frac{1}{2} & \\ \ddots & 1 & \\ & 0 & \\ & -1 & \ddots \\ & \frac{1}{2} & \ddots \\ & -\frac{1}{3} & \ddots \\ & \vdots & \end{pmatrix}.$$

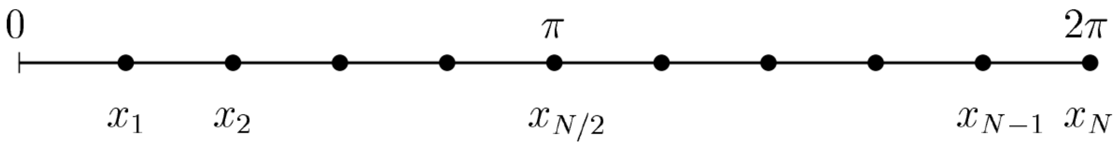
To construct a derivative matrix of higher order, we compute the derivative of $p(x)$ of the same order. For example,

$$S_h''(x_j) = \begin{cases} -\dfrac{\pi^2}{3h^2} & j = 0 \\ 2\dfrac{(-1)^{j+1}}{j^2h^2} & j \neq 0 \end{cases}$$

We obtain

$$D^2 v = \frac{2}{h^2} \begin{pmatrix} & \vdots & \\ \ddots & -\frac{1}{4} & \\ \ddots & 1 & \\ & -\frac{\pi^2}{6} & \\ & 1 & \ddots \\ & -\frac{1}{4} & \ddots \\ & \vdots & \end{pmatrix} v.$$

We consider the interval $[0, 2\pi]$. We discretize it with a uniform mesh of pitch $h = 2\pi/N$. We assume that N is even. We are only interested in periodic



functions v with period 2π. In this case, $\hat{v}$ is discrete, because only waves e^{ikx} with integer wavenumber k have period 2π. In this case,

$$\begin{array}{lcccl}
\text{Physical domain} & : & \text{discrete,} & \text{bounded} & : \; x \in \{h, 2h, ..., 2\pi - h, 2\pi\} \\
 & & \updownarrow & \updownarrow & \\
\text{Spectral domain} & : & \text{bounded,} & \text{discrete} & : \; k \in \left\{-\frac{N}{2} + 1, -\frac{N}{2} + 2, ..., \frac{N}{2}\right\}
\end{array}$$

Remember that

$$\frac{N}{2} = \frac{\pi}{h}$$

The Discrete Fourier Transform (DFT) is

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

The inverse transform is

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

To construct the interpolation function necessary for the calculation of the derivatives, we use the modified inverse transform. We define $\hat{v}_{-N/2} = \hat{v}_{N/2}$ and

$$p(x) = \frac{1}{2\pi} \left[\frac{1}{2} e^{-\frac{iNx}{2}} \hat{v}_{-N/2} + \sum_{k=-N/2}^{N/2} e^{ikx} \hat{v}_k + \frac{1}{2} e^{\frac{iNx}{2}} \hat{v}_{N/2} \right], \quad x \in [0, 2\pi].$$

This modification is necessary for the derivative to be a real function.

Note that $p(x)$ is a trigonometric polynomial of degree $N/2$, i.e., it can be written as a linear combination of the functions 1, $\sin(x)$, $\cos(x)$, $\sin(2x)$, $\cos(2x)$,...,$\cos(Nx/2)$.
We calculate $p(x)$ which corresponds to the periodic function δ,

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

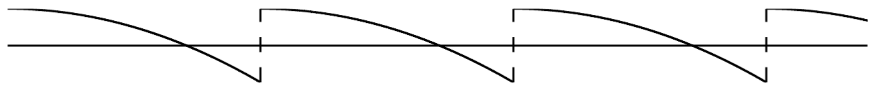
By the definition of the discrete Fourier transform, we obtain $\hat{\delta}_k = h$ for all k and

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

This function is called the periodic cardinal sine,

$$S_N(x) = \frac{\sin(\pi x/h)}{(2\pi/h)\tan(x/2)}.$$

We note that $S_N(x) \to S_h(x)$ in limit $x \to 0$.



We can develop a periodic function defined on the mesh based on translation of δ functions,

$$v_j = \sum_{m=1}^{N} v_m \delta_{j-m}.$$

We obtain the corresponding interpolating function,

$$p(x) = \sum_{m=1}^{N} v_m S_N(x - x_m).$$

To calculate the derivative of this function. We take note that

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

These numbers are the N-th column of the spectral differentiation matrix,

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

In the same way, we can calculate the second derivative,

$$S_N''(x_j) = \begin{cases} -\dfrac{\pi^2}{3h^2} - \dfrac{1}{6} & j = 0 \mod N \\ -\dfrac{(-1)^j}{2\sin^2(jh/2)} & j \neq 0 \mod N \end{cases}$$

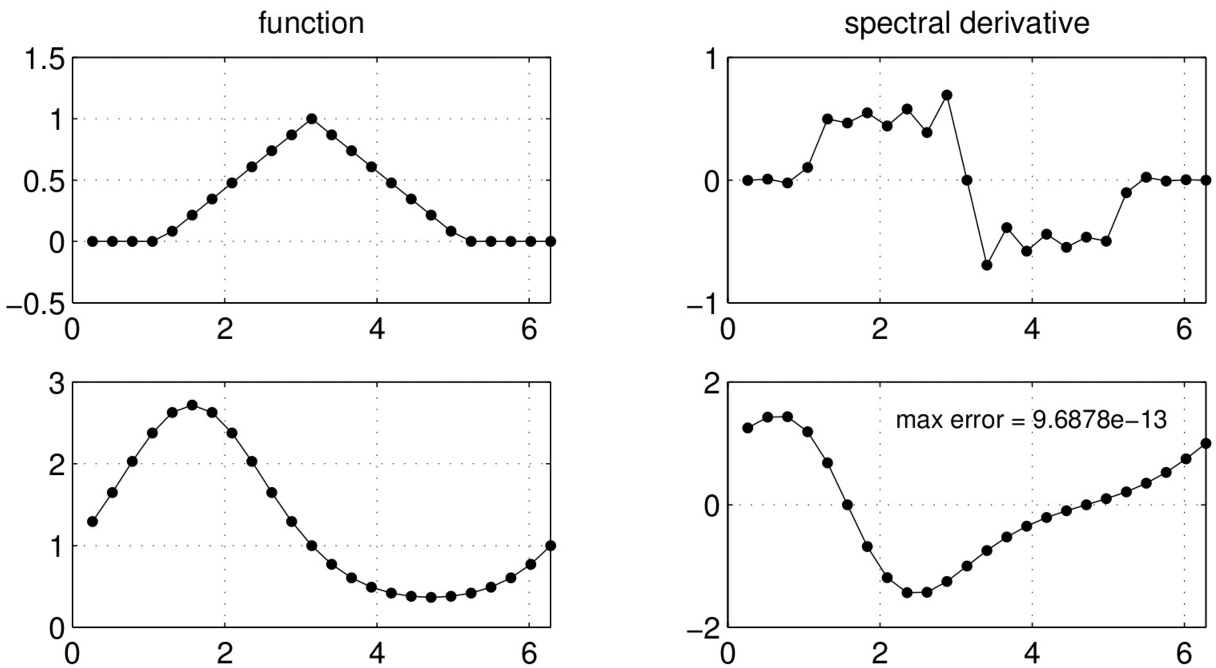
$$D_N^{(2)} = \begin{pmatrix} & \vdots & \\ \ddots & -\frac{1}{2}\csc^2\frac{2h}{2} & \\ \ddots & \frac{1}{2}\csc^2\frac{h}{2} & \\ & -\frac{\pi^2}{3h^2} - \frac{1}{6} & \\ & \frac{1}{2}\csc^2\frac{h}{2} & \ddots \\ & -\frac{1}{2}\csc^2\frac{2h}{2} & \ddots \\ & \vdots & \end{pmatrix}.$$

Exemple. Derivative of function $\max(0, 1 - \frac{|x-\pi|}{2})$ and function $e^{\sin(x)}$.

```
N = 24; h = 2*pi/N; x = h*(1:N)';
column = [0 .5*(-1).^(1:N-1).*cot((1:N-1)*h/2)]';
D = toeplitz(column,column([1 N:-1:2]));

v = max(0,1-abs(x-pi)/2); clf
subplot(3,2,1), plot(x,v,'.-','markersize',13)
axis([0 2*pi -.5 1.5]), grid on, title('function')
subplot(3,2,2), plot(x,D*v,'.-','markersize',13)
axis([0 2*pi -1 1]), grid on, title('spectral derivative')

v = exp(sin(x)); vprime = cos(x).*v;
subplot(3,2,3), plot(x,v,'.-','markersize',13)
axis([0 2*pi 0 3]), grid on
subplot(3,2,4), plot(x,D*v,'.-','markersize',13)
axis([0 2*pi -2 2]), grid on
error = norm(D*v-vprime,inf);
text(2.2,1.4,['max error = ' num2str(error)])
```


function
spectral derivative
max error = 9.6878e−13

We can also calculate the spectral derivative with the following algorithm

- Given v, calculate $\hat{v}$.
- Define $\hat{w}_k = ik\hat{v}_k$ and $\hat{w}_{N/2} = 0$.
- Calculate w from $\hat{w}$.

In the same way, we calculate the ν-th derivative,

- Given v, calculate $\hat{v}$.
- Define $\hat{w}_k = (ik)^\nu \hat{v}_k$ and $\hat{w}_{N/2} = 0$ if ν is even.
- Calculate w from $\hat{w}$.

These algorithms allow the use of *Fast Fourier Transform (FFT)*. This reduces the number of operations to $\mathcal{O}(N \log N)$.

```
N = 30; h = 2*pi/N; x = h*(1:N)';
v = max(0,1-abs(x-pi)/2); v_hat = fft(v);
w_hat = 1i*[0:N/2-1 0 -N/2+1:-1]' .* v_hat;
w = real(ifft(w_hat)); clf
subplot(3,2,1), plot(x,v,'.-','markersize',13)
axis([0 2*pi -.5 1.5]), grid on, title('function')
subplot(3,2,2), plot(x,w,'.-','markersize',13)
axis([0 2*pi -1 1]), grid on, title('spectral derivative')

v = exp(sin(x)); vprime = cos(x).*v;
v_hat = fft(v);
w_hat = 1i*[0:N/2-1 0 -N/2+1:-1]' .* v_hat;
w = real(ifft(w_hat));
subplot(3,2,3), plot(x,v,'.-','markersize',13)
axis([0 2*pi 0 3]), grid on
subplot(3,2,4), plot(x,w,'.-','markersize',13)
axis([0 2*pi -2 2]), grid on
error = norm(w-vprime,inf);
text(2.2,1.4,['max error = ' num2str(error)])
```

Smooth functions have the Fourier transform rapidly converging to zero in the limit $|k| \to \infty$. In this case, the discretization error is small because this error is due to the aliasing of the high wavenumbers to the resolved wavenumbers.

Theorem. Let $u \in L^2(\mathbb{R})$. $\hat{u}$ is the Fourier transform of u.

- If u has $p-1$ continuous derivatives in $L^2(\mathbb{R})$, where $p \geq 0$, and the p-th derivative is of bounded variation (in $L^1(\mathbb{R})$ and the supremum of $\int fg'$ is finite over all $g \in C^1(\mathbb{R})$, $|g(x)| \leq 1$), then
$$\hat{u}(k) = \mathcal{O}(|k|^{-p-1}), \qquad |k| \to \infty.$$
- If there exist $a, c > 0$ such that we can extend u and the extension is an analytic function on $|\Im z| < a$ with $||u(\cdot + iy)|| \leq c$ uniformly for all $y \in (-a, a)$, where $||u(\cdot + iy)||$ is the norm L^2 along the axis $\Im z = y$, then $e^{a|k|}\hat{u}(k) \in L^2(\mathbb{R})$. The converse is also true.
- If the extension of u is an analytic function everywhere in the complex plane and if there exists $a > 0$ such that $|u(z)| = o(e^{a|z|})$, $|z| \to \infty$, then $\hat{u}$ has

compact support,

$$\hat{u}(k) = 0 \qquad \text{for all } |k| > a.$$

The converse is also true.

Example. Consider a function

$$s(x) = \begin{cases} \frac{1}{2} & |x| \leq 1 \\ 0 & |x| > 1 \end{cases}$$

This function is discontinuous, but it has bounded variation. It verifies the conditions of the first part of the theorem with $p = 0$. Its Fourier transform is

$$\hat{s}(k) = \frac{\sin k}{k}.$$

Now consider a convolution

$$(s * s)(x) = \int_{-\infty}^{\infty} s(y)s(x-y)dy.$$

It is a piecewise linear function. It has compact support on $[-2, 2]$. It is continuous and its derivative has bounded variation. It verifies the conditions of the theorem with $p = 1$. Its Fourier transform is

$$\widehat{s * s}(k) = \left(\frac{\sin k}{k}\right)^2.$$

This formula is obtained by using the property of the Fourier transform of the convolution

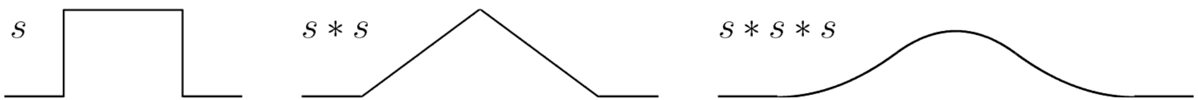
$$\widehat{u * v}(k) = \hat{u}(k)\hat{v}(k), \qquad k \in \mathbb{R}.$$

The function $s * s * s$ has its second derivative with bounded variation. It is piecewise quadratic. Its support is $[-3.3]$. It verifies the conditions of the theorem with $p = 2$.

Its Fourier transform is

$$\widehat{s * s * s}(k) = \left(\frac{\sin k}{k}\right)^3.$$

In these three examples, the decay rate of the Fourier transform is $\mathcal{O}(|k|^{-1})$, $\mathcal{O}(|k|^{-2})$ and $\mathcal{O}(|k|^{-3})$, respectively.



Example.

$$u(x) = \frac{\sigma}{x^2 + \sigma^2}, \qquad \hat{u}(k) = \pi e^{-\sigma|k|}, \qquad \sigma > 0.$$

This function has two poles, $\pm i\sigma$. The conditions of the second part of the theorem hold, with $a < \sigma$. We see that $\hat{u}$ decreases exponentially. The decay rate is equal to σ.

Example.

$$u(x) = e^{-x^2/2\sigma^2} \qquad \hat{u}(k) = \sigma\sqrt{\frac{\pi}{2}}e^{-\sigma^2 k^2/2}.$$

This function verifies the conditions of the second part of the theorem because it is analytic but it does not satisfy the conditions of the third part, because its rate of growth along the imaginary axis is faster than exponential. Therefore, $\hat{u}(k)$ decays faster than exponentially but its support is not compact.

Aliasing formula (Poisson summation formula).

Let $u \in L^2(\mathbb{R})$. Suppose its derivative has bounded variation. Let v be the function obtained by sampling u on a grid $h\mathbb{Z}$, $v_j = u(x_j)$. Then, for all $k \in [-\pi/h, \pi/h]$,

$$\hat{v}(k) = \sum_{j=-\infty}^{\infty} \hat{u}(k + 2\pi j/h),$$

Where $\hat{u}$ is the Fourier transform of u and $\hat{v}$ is the semi-discrete Fourier transform of v.
We see that

$$\hat{v}(k) - \hat{u}(k) = \sum_{j=-\infty,\quad j\neq 0}^{\infty} \hat{u}(k + 2\pi j/h),$$

the decay rate of $\hat{u}$ determines the decay rate of the error $\hat{v}(k) - \hat{u}(k)$ with $h \to 0$ for fixed k.

- If u has $p-1$ continuous derivatives in $L^2(\mathbb{R})$, where $p \geq 0$, and the p-th derivative has bounded variation, then

$$|\hat{v}(k) - \hat{u}(k)| = \mathcal{O}(h^{p+1}), \qquad h \to 0.$$

- If there exists $a, c > 0$ such that we can extend u and the extension is an analytic function on $|\Im z| < a$ with $||u(\cdot + iy)|| \leq c$ uniformly for all $y \in (-a, a)$, then

$$|\hat{v}(k) - \hat{u}(k)| = \mathcal{O}(e^{-\pi(a-\epsilon)/h}), \qquad h \to 0.$$

for all $\epsilon > 0$

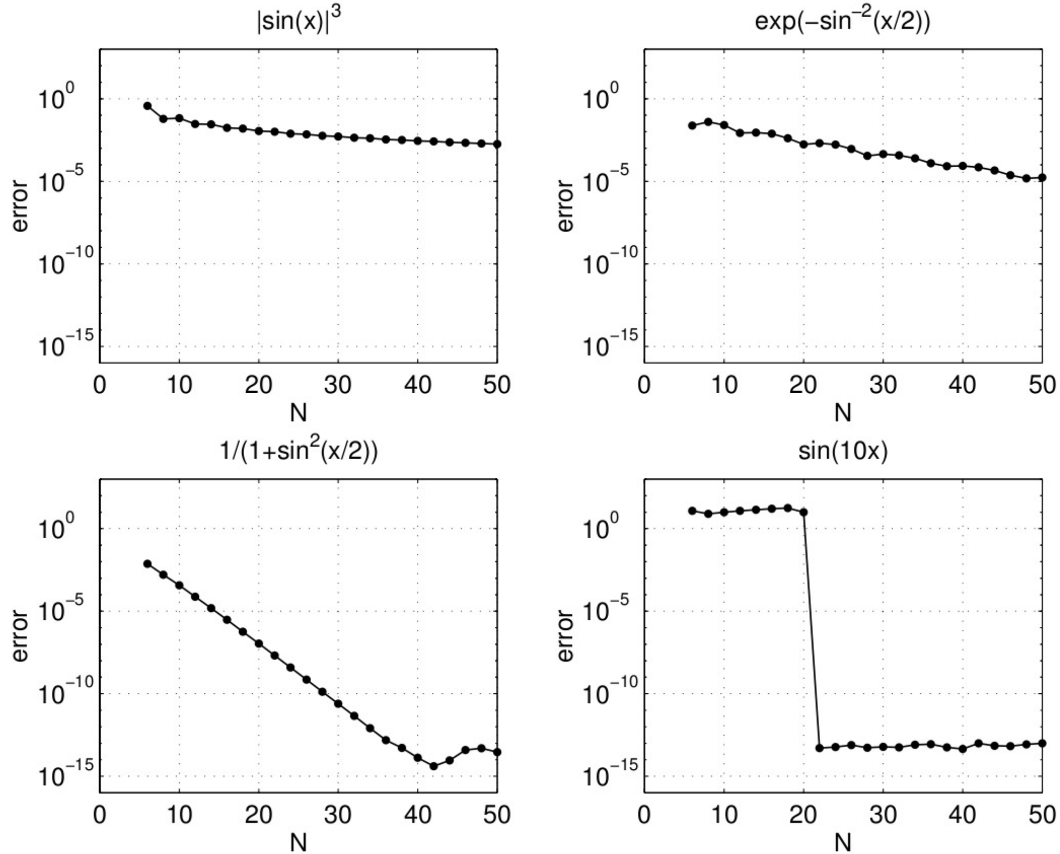
- If the extension of u is an analytic function everywhere in the complex plane and if there exists $a > 0$ such that $|u(z)| = o(e^{a|z|})$, $|z| \to \infty$, and if $h \leq \pi/a$, then
$$\hat{v}(k) = \hat{u}(k).$$

We use the Parseval equality to get

$$||u(x) - p(x)||_2 = \frac{1}{\sqrt{2\pi}}||\hat{u}(k) - \hat{v}(k)||_2$$

We obtain the error estimate for the ν-th spectral derivative

- If u has $p-1$ continuous derivatives in $L^2(\mathbb{R})$, where $p \geq \nu + 1$, and the p-th derivative has bounded variation, so
$$|w_j - u^{(\nu)}(x_j)| = \mathcal{O}(h^{p-\nu}), \qquad h \to 0.$$
- If there exists $a, c > 0$ such that we can extend u and the extension is an analytic function on $|\Im z| < a$ with $||u(\cdot + iy)|| \leq c$ uniformly for all $y \in (-a, a)$, so
$$|w_j - u^{(\nu)}(x_j)| = \mathcal{O}(e^{-\pi(a-\epsilon)/h)}), \qquad h \to 0.$$
for all $\epsilon > 0$
- If the extension of u is an analytic function everywhere in the complex plane and if there exists $a > 0$ such that $|u(z)| = o(e^{a|z|})$, $|z| \to \infty$, and if $h \leq \pi/a$, then
$$w_j = u^{(\nu)}(x_j).$$


|sin(x)|^3
exp(−sin^−2(x/2))
1/(1+sin^2(x/2))
sin(10x)
error
N
10^0
10^−5
10^−10
10^−15
0
10
20
30
40
50