SPECTRAL METHODS

Polynomial Approximation.

The expansion of a function 'u' in terms of an infinite sequence of orthogonal functions $\{\phi_k\}$, e.g., $u = \sum_{k=-\infty}^{\infty} \hat{u}_k \phi_k$ underlies many numerical methods of approximation.

↳ The accuracy of the approximations and the efficiency of their implementation influence decisively the domain of applicability of these methods in scientific computations.

- The most familiar approximation results are those for periodic functions expanded in Fourier series.

⇒ The k-th coefficient of the expansion decays faster than any inverse power of 'k' when the function is infinitely smooth and all its derivatives are periodic as well.

⇓

In practice this decay is not exhibited until there are enough coefficients to represent all the essential structures of the function. The subsequent rapid decay of the coefficients implies that the Fourier Series truncated after just a few more terms represents an exceedingly good approximation of the function.

⇓

SPECTRAL ACCURACY

+ usually spectral accuracy is attained (also with other non Fourier-type functions) when the function exhibits very special boundary behavior (e.g. eigenfunctions of a Sturm Liouville operator).

+ The expansion in terms of an orthogonal system introduces a linear transformation between "u" and the sequence of its expansion coefficients $\{\hat{u}_k\}$.

↳ The expansion coefficients depen on (almost) all the values of "u" in physical space, and they can rarely be computed exactly. A finite approximate expansion coefficients can be easily computed using the values of "u" at a finite number of selected points, usually the nodes of high-precision quadrature formulas.

↳ This procedure defines a <u>discrete transform</u> between the set of values of "u" at the quadrature points and the set of appsoximate, or discrete, coefficients.

↳ The finite series defined by the discrete transform is actually the interpolant of "u" at the quadrature nodes.

$$Su = \sum_{k=-\infty}^{\infty} \hat{u}_k \phi_k \quad \text{(Fourier series of "}u\text{").}$$

Define the polynomial: $P_N(x) = \sum_{k=-N/2}^{N/2} \hat{u}_k e^{ikx}$ (N-th order truncated Fourier series of "u").

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• The Continuous Fourier Expansion:

The set of functions $\phi_k(x) = e^{ikx}$ is an orthogonal system over the interval $(0, 2\pi)$, such that:

$$\int_0^{2\pi} \phi_k(x)\, \underset{\substack{\uparrow \\ \text{(complex conjugate)}}}{\phi_\ell^*(x)}\, dx = 2\pi\, \delta_{k\ell} = \begin{cases} 0 & \text{if } k \neq \ell \\ 2\pi & \text{if } k = \ell \end{cases}$$

And the Fourier coefficients are given by: $\hat{u}_k = \frac{1}{2\pi} \int_0^{2\pi} u(x)\, e^{-ikx}\, dx \; ; \; k = 0, \pm 1, \pm 2, \ldots$

↳ This relation associates with 'u' a sequence of complex numbers called the Fourier Transform of "u".

• The Fourier series of the function "u" is defined as: $Su = \sum_{k=-\infty}^{\infty} \hat{u}_k \phi_k$ and it represents the formal expansion of "u" in terms of the Fourier orthogonal system. ⇒ For this expansion to be rigorous:

1) Is the series convergent?
2) What's the relation between the series and "u"?
3) How fast does the series converge?

⇒ Basically we are interested on knowing how well is "u" approximated by the sequence of trigonometric polynomials

$$P_N u(x) = \underbrace{\sum_{k=-N/2}^{N/2} \hat{u}_k\, e^{ikx}}_{\text{"N degrees of freedom"}} \quad \text{as} \quad N \to \infty.$$

1) If "u" is continuous, periodic and of bounded variation on $[0, 2\pi]$, then 'Su' is uniformly convergent to "u".

$$\max_{x \in [0,2\pi]} |u(x) - P_N u(x)| \longrightarrow 0 \quad \text{as} \quad N \to \infty.$$

- If "u" is of bounded variation on $[0, 2\pi]$, then $P_N u(x)$ converges pointwise to $(u(x^+) + u(x^-))/2$ for any $x \in [0, 2\pi]$ (here $u(0^-) = u(2\pi^-)$)

- if "u" is continuous and periodic, then its Fourier series does not necessarily converge at every point $x \in [0, 2\pi]$.

The series 'Su' is said to be convergent in the mean to "u" if

$$\int_0^{2\pi} |u(x) - P_N u(x)|^2 \, dx \longrightarrow 0 \quad \text{as} \quad N \to \infty.$$

2) The rate of convergence of the Fourier series is shown from the fact that:

$$\max_{0 \le x \le 2\pi} |u(x) - P_N u(x)| \le \sum_{|k| \ge N/2} |\hat{u}_k|$$

which shows that the size of the error created by replacing "u" with its N-th order truncated Fourier Series depends upon how fast the Fourier coefficients go to zero. This in turn depends on the regularity of "u" in the domain $(0, 2\pi)$ and on the periodicity properties of "u".

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if "u" is m-times continuously differentiable in $[0, 2\pi]$ $(m \geq 1)$, and if $u^{(j)}$ is periodic for all $j \leq m-2$, then

$$\hat{u}_k = O(k^{-m}) \quad ; \quad k = \pm 1, \pm 2, \ldots$$

$\hookrightarrow$ meaning that $\hat{u}_k$ decays like $k^{-(m-1)}$.

Conclusions: the k-th Fourier coefficient of a function which is infinitely differentiable and periodic with all its derivatives on $[0, 2\pi]$ decays faster than any negative power of "k".

Yet: if a series has a finite rate of decay, $\hat{u}_k = O(k^{-m})$, then this decay is observed only for $k >$ some k_0. Should the series be truncated below 'k_0', then the approximation will be quite poor.

$\hookrightarrow$ Even for an infinitely differentiable function there is some minimum 'k_0' acceptable, and truncations below this level yield thoroughly unacceptable approximations.

- The discrete Fourier expansion: $\longrightarrow$ (We can not keep infinite number of terms)
($\int u(x) e^{ikx} dx \longrightarrow$ hard to evaluate).

Some times the Fourier coefficients of an arbitrary function are not known in closed form and must therefore be approximated in some way.

↳ Maybe the function 'u' is only known at a set of points x_j;

for $N > 0$, $x_j = \frac{2\pi j}{N}$ with $j = 0, \ldots N-1$ (nodes or grid points)

⇒ The discrete Fourier coefficients of a complex-valued function "u" in $[0, 2\pi]$ with respect to these points are

$$\tilde{u}_k = \frac{1}{N} \sum_{j=0}^{N-1} u(x_j)\, e^{-ikx_j} \quad \text{with } k = -N/2, \ldots, N/2 - 1$$

throughout space

Hence: $$I_N u(x) = \sum_{k=-N/2}^{N/2-1} \tilde{u}_k e^{ikx}$$

(through out space)

is the $N/2$-degree trigonometric interpolant of "u" at the nodes.
(also known as discrete Fourier Series of "u").

Note that $\tilde{u}_k$ only depends on the "N" values of "u" at the nodes.

↳ The discrete Fourier transform is the mapping between N complex numbers $u(x_j)$, $j = 0, \ldots, N-1$ and the N complex numbers $\tilde{u}_k$ with $k = -N/2, \ldots, N/2 - 1$.

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The discrete Fourier coefficients can be expressed also in terms of the exact Fourier coefficients of "u".

$$\tilde{u}_k = \hat{u}_k + \sum_{\substack{m \neq 0 \\ m=-\infty}}^{+\infty} \hat{u}_{k+Nm} \qquad k = -N/2, \ldots, N/2 - 1$$

↳ This reflects that the k-th mode of the trigonometric interpolant of "u" depends not only on the k-th mode of 'u', but also on all the modes of "u" that alias the k-th mode on the discrete grid. The $(k+Nm)$th wavenumber aliases the k-th wavenumber on the grid.

[illustrate Fig 2.2 from Canuto's Book]

⇒ This can be rewritten as: $I_N u = P_N u + \underbrace{R_N u}_{\text{Residu}}$

$$\text{with} \quad R_N u = \sum_{k=-N/2}^{N/2-1} \left(\sum_{\substack{m \neq 0 \\ m=-\infty}}^{\infty} u_{k+Nm} \right) \phi_k$$

The error '$R_N u$' between the interpolating polynomial and the truncated Fourier series is called the "aliasing error".

The error $R_N u$ between the interpolating polynomial and the truncated Fourier series is called the <u>aliasing error</u>, and it is orthogonal to the truncation error:

$$\underbrace{\| u - I_N u \|^2}_{\substack{\text{The interpolation}\\ \text{error is always}\\ \text{larger than the}\\ \text{error due to the}\\ \text{truncation of the}\\ \text{Fourier series}}} = \underbrace{\| u - P_N u \|}^2 + \| R_N u \|^2$$

- <u>Note</u> that it has been proven that the influence of aliasing on the accuracy of spectral methods is asymptotically of the same order as the truncation error. (The truncation & interpolation errors decay at the same rate).

  ↳ The influence of aliasing in errors in the resolution of PDE will be further explored later.

<u>Note</u>: The sequence of interpolating polynomials exhibits convergence properties similar to those of the sequence of truncated Fourier series; the discrete & continuous Fourier coefficients share the same asymptotic behavior.

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when $N \to \infty$,

a) if 'u' is continuous, periodic and of bounded variation on $[0, 2\pi]$, then $I_N u$ converges to 'u' uniformly on $[0, 2\pi]$

b) if 'u' is of bounded variation on $[0, 2\pi]$, then $I_N u$ is uniformly bounded on $[0, 2\pi]$ and converges pointwise to 'u' at every continuity point for 'u'.

c) if 'u' is Riemann integrable, then $I_N u$ converges to 'u' in the mean.

d) the asymptotic behavior of $\tilde{u}_k$ is similar to $\hat{u}_k$ under the same conditions.

• Differentiation:

In Fourier space if: $Su = \sum_{k=-\infty}^{\infty} \hat{u}_k \phi_k$ is the Fourier series of a function "u", then,

$Su' = \sum_{k=-\infty}^{\infty} ik\, \hat{u}_k \phi_k$ is the Fourier series of the derivative of "u".

Consequently: $(P_N u)' = P_N u'$ (truncation and differentiation commute).

Differentiation in physical space is based upon the values of the function "u" at the Fourier nodes $\left(x_j = \frac{2\pi j}{N}\right)$. These are used in the evaluation of the discrete Fourier coefficients of "u". These are then multiplied by "ik" and the resulting Fourier coefficients are then transformed back to physical space.

$$\text{Hence:} \quad \underbrace{D_N u}_{\text{Fourier interpolation derivative.}} = (I_N u)'$$

$$\neq$$

$P_N u'$ $\Rightarrow$ True spectral derivative of "u": "<u>Fourier projection derivative</u>"

<u>Problem:</u> interpolation & derivation do not commute $(I_N u)' \neq I_N(u')$

$\hookrightarrow$ Solution: (saves us in CFD) $\longrightarrow$ the error $(I_N u)' - I_N(u')$ is of the same order as the truncation error for the derivative: $u' - P_N u'$

$\Rightarrow$ it follows that "interpolation differentiation is spectrally accurate).

<u>Note:</u> From a computational point of view, the Fourier interpolation derivative can be evaluated, requiring N multiplications and two discrete Fourier transforms.

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The Gibbs Phenomenon (see figure)

Describes the characteristic oscillatory behavior of the truncated Fourier series or the discrete Fourier series of a function of bounded variation in the neighborhood of a point of discontinuity.

↓

Generally it appears when the discretization grid doesn't have enough resolution.

↳ The Gibbs phenomenon influences the behavior of the truncated Fourier series not only in the neighborhood of the point of singularity, but also over the entire interval $[0, 2\pi]$.

↓

There are smoothing functions. Since the Gibbs phenomenon is related to the slow decay of the Fourier coefficients of a discontinuous function, it is natural to use smoothing procedures that attenuate the higher order coefficients. ⇒ Thus the oscillations associated with the higher order modes in the trigonometric approximant are damped.

↳ Smoothed series: $$S_N u = \sum_{k=-N/2}^{N/2-1} \sigma_k \hat{u}_k e^{ikx}$$

with $\sigma_k = 1 - \dfrac{|k|}{(N/2+1)}$ → decays linearly with $|k|$

Figure representing Aliasing Errors:

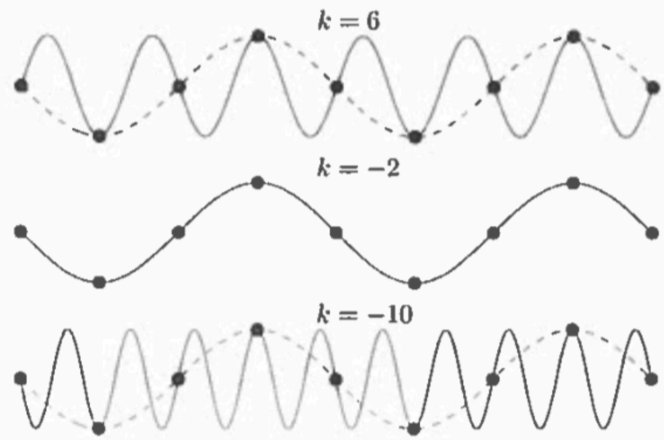

Fig. 2.2. Three sine waves that have the same $k = -2$ interpretation on an eight-point grid. The nodal values are denoted by the filled circles. The actual sine waves are denoted by the solid curves. Both the $k = 6$ and the $k = -10$ waves are misinterpreted as a $k = -2$ wave (dashed curves) on the coarse grid

Figure representing approximations of the derivatives:

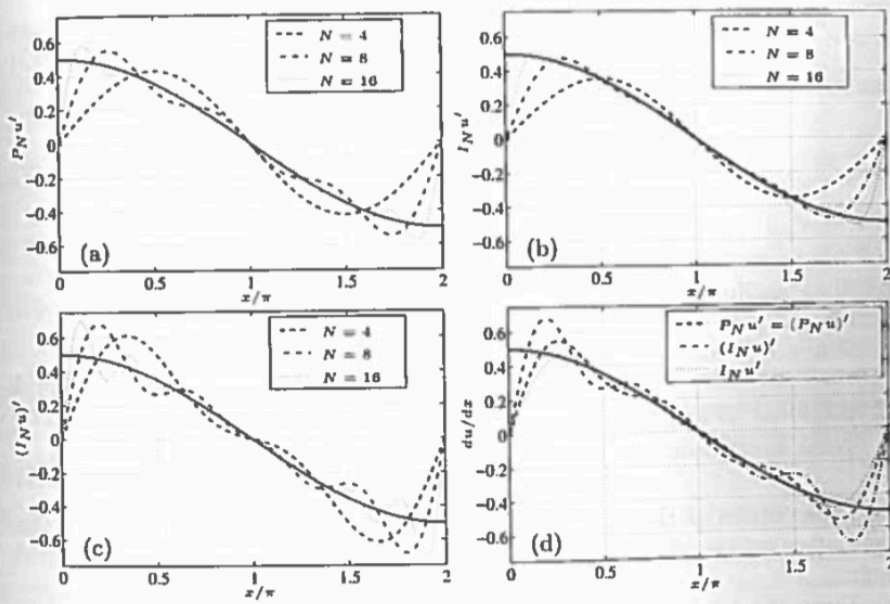

Fig. 2.3. Several versions of Fourier differentiation for $u(x) = \sin(x/2)$. The exact result is indicated by the solid curves and the approximate results for $N = 4$, 8 and 16 are indicated by the dashed curves. (a) $P_N u'$ and $(P_N u)'$; (b) $I_N u'$; (c) $(I_N u)'$. Part (d) shows all versions for $N = 8$

Figure representing Gibbs phenomena:

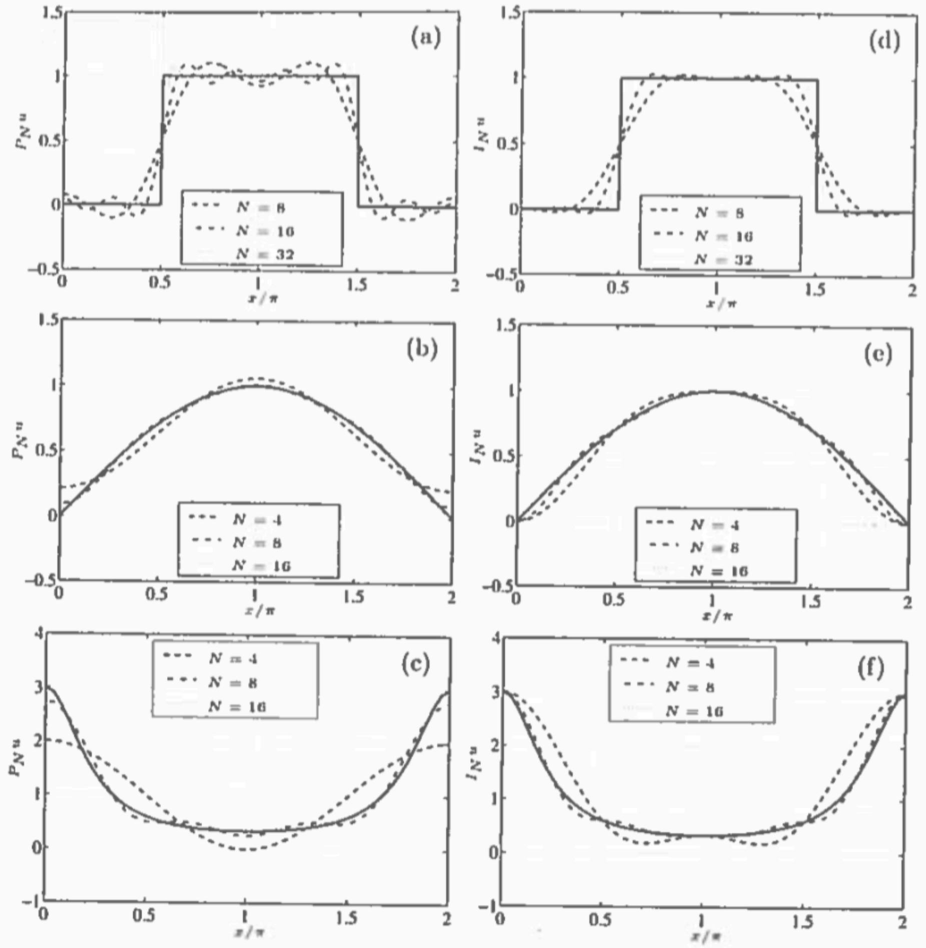

Fig. 2.1. Trigonometric approximations to the square wave ((a) and (d)), to $u(x) = \sin(x/2)$ ((b) and (e)) and to $u(x) = 3/(5 - 4\cos x)$ ((c) and (f)). Parts (a), (b), and (c) display truncated Fourier series. Parts (d), (e), and (f) display Fourier interpolating polynomials. The exact function is denoted by the solid curve