Spectral interpolation, differentiation and spectral methods for PDEs

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Spectral Interpolation

Define the DFT coefficients (on $[0, 2\pi]$)

$$c_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-ikx_j}, \quad k = -N/2, \ldots, N/2 - 1,$$

Then we have

$$f(x_j) = \sum_{k=-N/2}^{N/2-1} c_k e^{ikx_j}, \quad j = 0, \ldots, N-1.$$

Consider the function $\Pi_N f$,

$$\Pi_N f(x) = \sum_{k=-N/2}^{N/2-1} c_k e^{ikx}, \quad x \in \mathbb{R}.$$

This is an interpolating trigonometric polynomial, the so-called *spectral interpolant*.
Note: Instead using the coefficients c_k, $k = 0, \ldots, N-1$ and an interpolant based on this yields a BAD interpolant, see HW5.
Even for real f, this interpolant is in general complex (with the exception of the grid points x_j, of course).

Spectral Interpolation (cont.)

- If $c_{-N/2}$ has a non-zero imaginary part, then $\Pi f(x)$ is not a real-valued function, even if $f(x)$ is real valued.
- Set $c_{-N/2} = 0$ s.t.

$$\Pi_N f(x) = \sum_{k=-N/2}^{N/2-1} c_k e^{ikx} = \sum_{k=-N/2+1}^{N/2-1} c_k e^{ikx}.$$

  With this definition, $\Pi f(x)$ is a real valued function!
  (if $f(x)$ is real valued)
- Show it!
- This is a global procedure. All grid values f_j will contribute to each interpolated value.

Fourier coefficients and DFT coefficients

Now, let us distinguish between the Fourier coefficients for $f(x)$ on $[0, 2\pi]$ as defined by

$$\hat{f}_k = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-ikx} dx,$$

and the DFT coefficients as defined by
(with $f_j = f(x_j)$, $x_j = jh$, $h = 2\pi/N$),

$$\tilde{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-ikx_j}, \quad k = -N/2, \ldots, N/2-1.$$

Define the truncated Fourier series and the interpolant based on the DFT coefficients:

$$P_N f(x) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k e^{ikx}, \qquad \Pi_N f(x) = \sum_{k=-N/2}^{N/2-1} \tilde{f}_k e^{ikx}.$$

Define the full Fourier series by

$$Sf(x) = \sum_{k=-\infty}^{\infty} \hat{f}_k e^{ikx}.$$

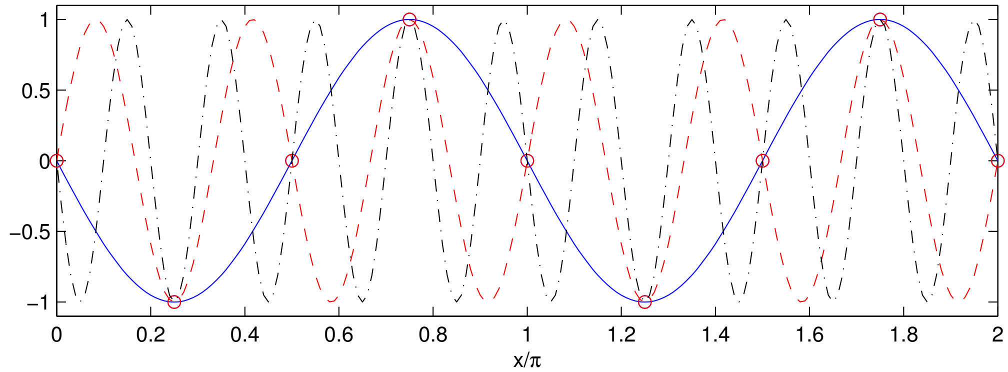
Fourier coefficients and DFT coefficients, contd

- Assuming that Sf converges to f, we get [NOTES]

$$\tilde{f}_k = \hat{f}_k + \sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \hat{f}_{k+mN}, \quad k = -N/2, \dots, N/2-1$$

- The $(k+Nm)^{th}$ frequency aliases the kth frequency on the grid.
- They are indistinguishable at the nodes since $e^{ikx_j} = e^{i(k+mN)x_j}$.

Example: Plotting $\sin(-2x)$, $\sin(6x)$ and $\sin(-10x)$.
For $N = 8$, they all coincide at grid points.



Aliasing errors

- We can now write

$$\Pi_N f(x) = P_N f(x) + R_N f(x),$$

where the error $R_N f$ between the interpolating polynomial and the trunctated Fourier series is called "aliasing error", and is given by

$$R_N f = \sum_{k=-N/2}^{N/2-1} \left(\sum_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \hat{f}_{k+mN} \right) e^{ikx}.$$

- The aliasing error $R_N f$ is orthogonal to the truncation error $f - P_N f$, and so

$$\|f - \Pi_N f\|^2 = \|f - P_N f\|^2 + \|R_N f\|^2$$

- However, the sequence of interpolating polynomials exhibits convergence properties similar to those of the sequence of truncated Fourier series.
- Furthermore, the continuous and discrete Fourier coefficients share the same asymptotic behavior (decay of coefficients).

Differentiation

Idea: Given a function u at discrete points, interpolate by a suitable smooth function $p(x)$ and set $u'(x_j) \approx p'(x)$.
Examples:

- Piecewise linear interpolation: $u'(x_j) \approx \dfrac{u_{j+1} - u_j}{h}$
- Piecewise quadratic interpolation: $u'(x_j) \approx \dfrac{u_{j+1} - u_{j-1}}{2h}$

Let's now use spectral interpolation:

$$f^{(p)}(x_j) \approx \frac{d^p}{dx^p} \Pi_N f(x)|_{x=x_j} = \sum_{k=-N/2}^{N/2-1} \tilde{f}_k \left[\frac{d^p}{dx^p} e^{ikx} \right]_{x=x_j} = \sum_{k=-N/2}^{N/2-1} \tilde{f}_k \cdot (ik)^p e^{ikx_j},$$

where $\tilde{f}_k$ are the DFT coefficients for $f(x)$.
Remarks:

- Piecewise polynomial interpolation uses only *local* informations.
- Spectral differentiation uses all gridpoints for evaluating one derivative.
- Computational complexity:
  Polynomial: $O(N)$, Spectral via FFT: $O(N \log N)$.

Accuracy of differentiation

- For piecewise polynomial approximation, the accuracy depends on the order and the grid size. I.e. with $h = 2\pi/N$, errors proportional to h^1 or h^2, etc. (Assuming the function is smooth enough, not much regularity required).
- For spectral differentiation, the convergence depends on N and on the smoothness of the function.
- As discussed before, the smoother f is, the faster does it's Fourier coefficients decay. Also true for the discrete Fourier coefficients.
- If f is infinitely smooth and periodic with all its derivatives, $\tilde{f}_k$ decays faster than algebraically in k^{-1}.
- Slower decay for each additional derivative, since Fourier coefficient is $(ik)^p \tilde{f}_k$ for $f^{(p)}(x)$.

Spectral methods for differential equations

An example:
Find the 2π-periodic solutions of

$$-u'' + ru = f(x), \quad x \in (0, 2\pi)$$

with a *constant* $r > 0$.
Weak formulation, with $V = H^1_{\text{per}}(0, 2\pi)$:
Find $u \in V$ such that

$$a(u, v) = L(v), \quad \forall v \in V,$$

where

$$a(u, v) = \int_0^{2\pi} (u'\bar{v}' + ru\bar{v})dx, \quad L(v) = \int_0^{2\pi} f\bar{v}dx.$$

Introduce the Fourier expansion of u,

$$u(x) = \sum_{k=-\infty}^{\infty} \hat{u}_k e^{ikx} = \sum_{k=-\infty}^{\infty} \hat{u}_k \phi_k(x), \text{ with } \phi_k(x) = e^{ikx}.$$

Analytic solution

Remember the orthogonality condition:

$$\int_0^{2\pi} \phi_k(x)\bar{\phi}_\ell(x)dx = \int_0^{2\pi} e^{ikx}e^{-i\ell x}dx = 2\pi\delta_{k\ell},$$

where $\delta_{k\ell}$ is the Kronecker delta.
Insert the Fourier expansion and test against *all* basis functions $\phi_\ell = e^{i\ell x}$:

$$a(u, \phi_\ell) = \int_0^{2\pi} \left(\sum_{k=-\infty}^{+\infty} ik\hat{u}_k e^{ikx}\overline{i\ell e^{i\ell x}} + r \sum_{k=-\infty}^{+\infty} \hat{u}_k e^{ikx}\overline{e^{i\ell x}} \right)dx$$
$$= \sum_{k=-\infty}^{+\infty} \hat{u}_k \int_0^{2\pi} (ik \cdot (-i\ell) + r)e^{i(k-\ell)x}dx = 2\pi\hat{u}_\ell(\ell^2 + r).$$

Similarly,

$$L(v) = \int_0^{2\pi} f(x)e^{-i\ell x}dx = 2\pi\hat{f}_\ell.$$

Hence,

$$\boxed{\hat{u}_k = \frac{1}{j^2 + r}\hat{f}_k, \quad k = 0, \pm 1, \pm 2, \ldots}$$

About the analytic solution

The example was: find the 2π-periodic solutions of

$$-u'' + ru = f(x), \quad x \in (0, 2\pi), \text{ with a } \textit{constant } r > 0,$$

and the Fourier coefficients for u can be determined in terms of the Fourier coefficients for f,

$$\boxed{\hat{u}_k = \frac{1}{j^2 + r}\hat{f}_k, \quad k = 0, \pm 1, \pm 2, \dots}.$$

- If $r = 0$, would divide by 0 for $k = 0$. In this case, Eq. and BC only determines u up to a constant: If u is a solution, so is $u + C$. Natural to require, $\hat{f}_0 = 0$ (i.e. $\int_0^{2\pi} f(x)dx = 0$).
- If $f \in H^p_{\text{per}}(0, 2\pi)$, then $u \in H^{p+2}_{\text{per}}(0, 2\pi)$:

$$\sum_{k=-\infty}^{+\infty} k^{2p+4}|\hat{u}_k|^2 = \sum_{k=-\infty}^{+\infty} k^{2p+4}\frac{|\hat{f}_k|^2}{(k^2+r)^2} < \sum_{k=-\infty}^{+\infty} k^{2p}|\hat{f}_k|^2 < \infty$$

Galerkin's method

Apply now Galerkin's method with $V_N = \{v | v = \sum_{k=-N/2}^{N/2} \hat{v}_k e^{ikx}\}$:

Introduce an expansion of $u \in V_N$,

$$u(x) = \sum_{k=-N/2}^{N/2} \hat{u}^N_k e^{ikx}.$$

If we assume an truncated Fourier expansion of f (coeffs still the continuous Fourier coefficients),

$$f(x) = \sum_{k=-N/2}^{N/2} \hat{f}_k e^{ikx},$$

then, similarly to the infinite expansion, we get:

$$\boxed{\hat{u}^N_k = \frac{1}{j^2 + r}\hat{f}_k, \quad k = 0, \pm 1, \pm 2, \dots}, \quad \text{i.e. } \boxed{\hat{u}^N_k = \hat{u}_k}$$

Error analysis: Galerkin's method

Error estimation:

$$e_N(x) = u(x) - u_N(x) = \sum_{|k|>N/2} \hat{u}_k e^{ikx}$$

Theorem

- For all square integrable functions f,

$$\boxed{\|e_N\| \leq \frac{4}{N^2}\|f\|}$$

(quadratic convergence).

- If $f \in H^p_{\text{per}}(0, 2\pi)$:

$$\boxed{O\left(N^{-(p+1)}\right)}.$$

- If $f \in C^\infty$, we have exponential convergence.

Error analysis: Proofs

- For $f \in L^2(0, 2\pi)$,

$$\|e_N\|^2 = 2\pi \sum_{|k|>N/2} |\hat{u}_k|^2 = 2\pi \sum_{|k|>N/2} \frac{|\hat{f}_k|^2}{(k^2+r)^2}$$
$$\leq \frac{1}{(N^2/4+r)^2}\|f\|^2 \leq \frac{16}{N^4}\|f\|^2$$

- If $f \in H^p_{\text{per}}(0, 2\pi)$:

$$\|e_N\|^2 = 2\pi \sum_{|k|>N/2} \frac{|\hat{f}_k|^2}{(k^2+r)^2} = 2\pi \sum_{|k|>N/2} \frac{k^{2p}}{k^{2p}} \frac{|\hat{f}_k|^2}{(k^2+r)^2}$$
$$\leq \frac{2\pi}{(N/2)^{2p}(N^2/4+r)^2} \sum_{|k|>N/2} k^{2p}|\hat{f}_k|^2 \leq \frac{C(p)^2}{N^{2p+2}}$$

Galerkin's method in practice

- Due to the structure of the FFT method, most efficient when N even, and preferably even $N = 2^m$.
- Therefore, one normally uses expansions.

$$u(x) = \sum_{k=-N/2}^{N/2-1} \hat{u}_k e^{ikx}.$$

- To make sure that the function stays real valued if all coefficients and initial conditions are real valued, one would set $\hat{u}_{-N/2} = 0$. Compare to interpolation.
- Error results on last few slides based on continuous Fourier coeffs. But in practice, will have DFT coeffs. Similar results.

Collocation method

- Consider again the equation $-u'' + ru = f$.
- Ansatz as before $u_N = \sum_{k=-N/2}^{N/2-1} c_k e^{ikx}$.
- Collocation: Use test functions $v_j(x) = \delta(x - x_j)$ for $x_j = jh - \pi$, $h = 2\pi/N$. Equivalently,

$$-u_N''(x_j) + ru_N(x_j) = f(x_j), \quad j = -N/2, \dots, N/2 - 1.$$

- Insert expansion and enforce this pointwise equality:

$$\sum_{k=-N/2}^{N/2-1} [c_k(k^2 + r) - \hat{f}_k]e^{ikx_j} = 0, \text{ all } j$$

$$\implies \quad c_k(k^2 + r) - \hat{f}_k = 0, \quad \text{all } k$$

- The solution becomes

$$c_k = \frac{\hat{f}_k}{k^2 + r}.$$

This is the same solution as obtained by the Galerkin method.

Spectral methods for PDEs

- The Galerkin/Collocation approach can also be used for time-dependent problems.
- Expand

$$u^N(x) = \sum_{k=-N/2}^{N/2-1} \hat{u}_k(t) e^{ikx}.$$

  where the Fourier coefficients now depend on time.
  Similarly, expand any given function in the right hand side and the given initial conditions.
- Example: The heat equation with periodic boundary conditions,

$$u_t + cu_{xx} = 0, \quad u(0,t) = u(2\pi, t), \quad u(x,0) = f(x)$$

  yields

$$\frac{d}{dt}\hat{u}_k + ck^2\hat{u}_k^2 = 0, \quad \hat{u}_k(0) = \hat{f}_k \quad -N/2 \leq k < N/2$$

  That is, we get an ODE for each Fourier coefficient.
- Time step in Fourier space, transform back to real space when solution is needed.

Non-linear PDEs - Galerkin's method

Consider Burger's equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0$$

Expanding u as u^N, multiply by a test function and integrate, and using orthogonality of the complex exponentials, we get

$$\frac{d}{dt}\hat{u}_k + \left(\widehat{u^N\frac{\partial u^N}{\partial x}}\right)_k + \nu k^2\hat{u}_k = 0, \qquad k = -N/2, \ldots, N/2-1$$

where

$$\left(\widehat{u^N\frac{\partial u^N}{\partial x}}\right)_k = \frac{1}{2\pi}\int_0^{2\pi} u^N\frac{\partial u^N}{\partial x}e^{-ikx}dx$$

is the kth Fourier coefficient for the nonlinear term.
For non-linear PDEs, the collocation approach and Galerkin approach might not coincide.

Non-linear term

- Consider a term $w(x) = u(x)v(x)$.
- We have that

$$\hat{w}_k = \widehat{(uv)}_k = \frac{1}{2\pi}\int_0^{2\pi} uve^{-ikx}dx$$

which yields

$$\widehat{(uv)}_k = \sum_{m+n=k} \hat{u}_m\hat{v}_n, \quad -N/2 \le k, m, n < N/2$$

- Convolution sum. Straightforward evaluation requires $O(N^2)$ operations.
- Idea of **pseudospectral** treatment:
  - Transform $\hat{u}_m$ and $\hat{v}_n$ to physical (real) space by IFFT.
  - Perform a multiplication in real space.
  - Transform to Fourier space by FFT to obtain $\hat{w}_k$.

Aliasing errors for pseudospectral treatment

Introduce the discrete transforms

$$U_j = \sum_{k=-N/2}^{N/2-1} \hat{u}_k(t)e^{ikx_j}, \quad V_j = \sum_{k=-N/2}^{N/2-1} \hat{v}_k(t)e^{ikx_j}, \quad j = 0, 1, \dots, N-1,$$

and define

$$W_j = U_jV_j, \quad j = 0, 1, \dots, N-1,$$

and

$$\hat{W}_k = \frac{1}{N}\sum_{j=0}^{N-1} W_je^{-ikx_j}, \quad k = -N/2, \dots, N/2-1$$

where $x_j = 2\pi j/N$.
Use of the discrete orthogonality condition leads to

$$\hat{W}_k = \sum_{m+n=k} \hat{u}_m\hat{v}_n + \sum_{m+n=k\pm N} \hat{u}_m\hat{v}_n = \hat{w}_k + \underbrace{\sum_{m+n=k\pm N} \hat{u}_m\hat{v}_n}_{\text{Aliasing error}}$$

Removal of aliasing errors by padding

Introduce M where $M > N$. Introduce the discrete transforms

$$U_j = \sum_{k=-M/2}^{M/2-1} \tilde{u}_k(t) e^{ikx_j}, \quad V_j = \sum_{k=-M/2}^{M/2-1} \tilde{v}_k(t) e^{ikx_j}, \quad j = 0, 1, \ldots, M-1,$$

and define

$$W_j = U_j v_j, \quad j = 0, 1, \ldots, M-1,$$

where $y_j = 2\pi j/M$, and

$$\tilde{u}_k = \begin{cases} \hat{u}_k & \text{if } -N/2 \leq k < N/2, \\ 0, & \text{otherwise.} \end{cases} \qquad \tilde{v}_k = \begin{cases} \hat{v}_k & \text{if } -N/2 \leq k < N/2, \\ 0, & \text{otherwise.} \end{cases}$$

Let

$$\tilde{W}_k = \frac{1}{M} \sum_{j=0}^{M-1} W_j e^{-iky_j}, \quad k = -M/2, \ldots, M/2-1.$$

If we define:

$$\hat{W}_k = \tilde{W}_k, \quad k = -N/2, \ldots, N/2-1,$$

and $M \geq 3N/2$, then the aliasing errors are removed.

Integrating factor technique

Consider the ODE

$$\frac{d}{dt}\hat{u}_k + \nu k^2 \hat{u}_k = \hat{F}_k$$

This yields

$$\frac{d}{dt}\left[e^{\nu k^2 t}\hat{u}_k\right] = e^{\nu k^2 t}\hat{F}_k$$

Discretize

$$\frac{e^{\nu k^2 (t_n + \Delta t)}\hat{u}_k^{n+1} - e^{\nu k^2 t_n}\hat{u}_k^n}{\Delta t} = e^{\nu k^2 t_n}\hat{G}_k^n$$

or, dividing through by $e^{\nu k^2 (t_n + \Delta t)}$,

$$\hat{u}_k^{n+1} = e^{-\nu k^2 \Delta t}\left(\hat{u}_k^n + \Delta t \hat{G}_k^n\right)$$

where $\hat{G}_k^n$ is a combination of different $\hat{F}_k$:s depending on the time-stepping method.
Example: For Forward Euler, $\hat{G}_k^n = \hat{F}_k^n$,
for the third order Adams Bashforth method (AB3),
$\hat{G}_k^n = \frac{1}{12}\left(23\hat{F}_k^n - 16\hat{F}_k^{n-1} + 5\hat{F}_k^{n-2}\right)$.

Non-linear PDEs - Collocation method

Again, consider Burger's equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0,$$

and expand u as u^N.
For the collocation method, we require that u^N staisfies the equation at $x_j = 2\pi j/N$, $j = 0, \ldots, N-1$, i.e. that

$$\left.\frac{\partial u^N}{\partial t} + u^N\frac{\partial u^N}{\partial x} - \nu\frac{\partial^2 u^N}{\partial x^2}\right|_{x=x_j} = 0.$$

This is discretized by

$$\left.\frac{\partial u^N}{\partial t} + u^N\mathcal{D}_N u^N - \nu\mathcal{D}_N^2 u^N\right|_{x=x_j} = 0,$$

where $\mathcal{D}_N$ is the Fourier collocation differentiation operator.

$$(\mathcal{D}_N u)_\ell = \sum_{k=-N/2}^{N/2-1} a_k e^{2\pi i k\ell/N}, \quad a_k = \frac{ik}{N}\sum_{j=0}^{N-1} u_j e^{-2\pi i kj/N}.$$

Collocation method for Burger's equation

Introducing vector notation,
$U(t) = (u^N(x_0, t), u^N(x_1, t), \ldots, u^N(x_{N-1}, t))$,
the discretized equation reads:

$$\frac{\partial U}{\partial t} + U \cdot D_N U - \nu D_N^2 U = 0,$$

where the $\cdot$ means pointwise multiplication and D_N is the matrix that represents the differentiation.
Starting from a different but equivalent form of Burger's equation:

$$\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial}{\partial x}(u^2) - \nu\frac{\partial^2 u}{\partial x^2} = 0,$$

the collocation discretization becomes,

$$\frac{\partial U}{\partial t} + \frac{1}{2}D_N(U \cdot U) - \nu D_N^2 U = 0.$$

These two discretizations are not equivalent, even if the two forms of the PDE are.

Comments on time-stepping

- For linear PDEs, taking the Galerkin view point, and solving ODEs for the Fourier coefficients, one needs to transform back to physical space only when the solution is needed, and not in each time step. Very cheap!
- For non-linear PDEs, both with a pseudo-spectral treatment in the Galerkin approach, or using the collocation formulation, FFTs will be needed in each time step to go in between physical space and real space.

(Pseudo) spectral methods - Summary

- Exponential convergence for smooth data. Very few degrees of freedom needed for high accuracy.
- Global basis functions. Cf FEM with local basis functions. Stiffness matrix full compared to sparse.
- FFTs used to accelerate computations.
- Computational cost $O(N \log N)$ per time step, where N is number of Fourier modes.
- Use of integrating factor to remove stiffness from ODEs in Fourier space, i.e. to relax CFL condition on explicit schemes.
- Aliasing errors arise from pseudo-spectral treatment of nonlinear terms. Can be removed by e.g. padding to the cost of a factor of 3/2 larger FFTs.
- Inflexible in terms of geometry. BCs see next slide.

(Pseudo) spectral methods - Non-periodic boundary conditions

- Fourier series are only well-suited for periodic boundary conditions.
- In case of Dirichlet boundary conditions, Chebyshev polynomials can be used (Strang, p. 465),

$$T_k(x) = \cos k\theta, \quad \text{with } \theta = \arccos x$$

- The Chebyshev polynomials are orthogonal over $-1 \leq x \leq 1$, if the inner product is defined using a weight function $w(x) = 1/\sqrt{1-x^2}$.
- The Chebyshev expansion of a function $u \in L^2_w(-1,1)$ is

$$u(x) = \sum_{k=0}^{\infty} \hat{u}_k T_k(x), \quad \hat{u}_k = \frac{2}{\pi c_k} \int_{-1}^{1} u(x) T_k(x) w(x) dx,$$

  where $c_0 = 2$ and $c_k = 1$, $k \geq 1$.
- The quadrature points are taken e.g. as the Gauss-Lobatto points, $x_j = cos \frac{\pi j}{N}$, $j = 0, \ldots, N$.
  Then the Fast Fourier Transform can be applied in the computations.