Numerical Methods II, Spring 2019
Spectral Methods

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1 Spectral methods for periodic KdV

These are excerpts from student solutions to the first two homeworks. In these notes we assume that the FFT convention is as defined in my lecture notes, that is, the one that corresponds to the formulas for Fourier series discretized with a trapezoidal rule (so factor $1/N$ in the forward transform but no factor in the inverse). The focus here is on handling the unmatched mode carefully.

1.1 interpft

Here N is number of nodes for Fourier approximation, and $M > N$ is number of fine nodes and we allow for arbitrary L.

We often consider the Fourier interpolation in the standard interval 2π, for now, we need to transfer to general length of interval L. The Fourier interpolation of $\phi(x)$ can be written as

$$\tilde{\phi}(x) = \begin{cases} \hat{\phi}_0 + \sum\limits_{0<k<\frac{N-1}{2}} \left(\hat{\phi}_k \exp(i\frac{2\pi}{L}kx) + \hat{\phi}_{N-1-k} \exp(-i\frac{2\pi}{L}kx) \right), \ N \text{ odd}, \\ \hat{\phi}_0 + \sum\limits_{0<k<\frac{N}{2}} \left(\hat{\phi}_k \exp(i\frac{2\pi}{L}kx) + \hat{\phi}_{N-k} \exp(-i\frac{2\pi}{L}kx) \right) + \hat{\phi}_{N/2} \cos(\frac{2\pi}{L}\frac{N}{2}x), \ N \text{ even}, \end{cases} \tag{1}$$

where N is the number of interpolation points and $\hat{\phi}_k$ are Fourier coefficients evaluated at interpolation grids $\frac{Lj}{N}, \ j = 0, \ldots, N-1$.

$$\hat{\phi}_k = \frac{1}{N} \sum_{j=0}^{N-1} \phi(\frac{Lj}{N}) \exp(-i\frac{2\pi}{L}k\frac{Lj}{N}) = \frac{1}{N} \sum_{j=0}^{N-1} \phi_j \exp(-i\frac{2\pi jk}{N}), \tag{2}$$

which stays the same as in the standard 2π interval.

On finer grids, we want to estimated our interpolation at $x_j = \frac{Lj}{M}$ $j = 0, \ldots, M-1, M \gg N$. The estimation can be written as

$$\tilde{\phi}(x_j) = \begin{cases} \hat{\phi}_0 + \sum\limits_{0<k<\frac{N-1}{2}} \left(\hat{\phi}_k \exp(i\frac{2\pi j}{M}k) + \hat{\phi}_{N-1-k} \exp(-i\frac{2\pi j}{M}k) \right), \ N \text{ odd}, \\ \hat{\phi}_0 + \sum\limits_{0<k<\frac{N}{2}} \left(\hat{\phi}_k \exp(i\frac{2\pi j}{M}k) + \hat{\phi}_{N-k} \exp(-i\frac{2\pi j}{M}k) \right) + \hat{\phi}_{N/2} \cos(\frac{2\pi j}{M}\frac{N}{2}), \ N \text{ even}, \end{cases} \tag{3}$$

which is still the same as in the standard 2π interval.

For the special $\frac{N}{2}$ mode when N is even, we can write

$$\hat{\phi}_{N/2} \cos(\frac{2\pi j}{M}\frac{N}{2}x) = \frac{\hat{\phi}_{N/2}}{2} \exp(i\frac{2\pi j}{M}\frac{N}{2}) + \frac{\hat{\phi}_{N/2}}{2} \exp(-i\frac{2\pi j}{M}\frac{N}{2}), \tag{4}$$

i.e separating the $\hat{\phi}_{N/2}$ into two halves and giving one half to the matched mode of $N/2$ in the finer grids.

So the routine of our Fourier Interpolations on a length-L interval is:

- If N is odd,
  1. Use `fft` on the N interpolation points to obtain Fourier coefficients $\hat{\phi}_0, \cdots, \hat{\phi}_{N-1}$;
  2. Apply oversampling to the Fourier coefficients
     $(\hat{c}_k)_{k=1}^N = (\hat{\phi}_0, \hat{\phi}_1, \cdots, \hat{\phi}_{(N-1)/2}, 0, \cdots, 0, \hat{\phi}_{(N-1)/2}, \cdots, \hat{\phi}_{n-1})$;
  3. Apply `ifft` to $(\hat{c}_k)_{k=1}^N$, obtain the interpolation estimated on fine grids.
- If N is even,
  1. Use `fft` on the N interpolation points to obtain Fourier coefficients $\hat{\phi}_0, \cdots, \hat{\phi}_{N-1}$;
  2. Apply oversampling to the Fourier coefficients
     $(\hat{c}_k)_{k=1}^N = (\hat{\phi}_0, \hat{\phi}_1, \cdots, \hat{\phi}_{N/2-1}, \frac{\hat{\phi}_{N/2}}{2}, 0, \cdots, 0, \frac{\hat{\phi}_{N/2}}{2}, \hat{\phi}_{N/2+1}, \cdots, \hat{\phi}_{N-1})$;
  3. Apply `ifft` to $(\hat{c}_k)_{k=1}^N$, obtain the interpolation estimated on fine grids.

1.2 Spectral Differentiation

Here n is number of nodes for Fourier approximation, and $N > n$ is number of fine nodes, and we assume $L = 2\pi$.

And for even n, there is unmatched mode corresponding to frequency $n/2$, so we use minimal oscillation trigonometric interpolation,

$$\phi(x) = \hat{f}_0 + \sum_{0<k<\frac{n}{2}} \left(\hat{f}_k e^{ikx} + \hat{f}_{n-k} e^{-ikx} \right) + \hat{f}_{n/2} \cos(\frac{nx}{2}), \tag{5}$$

where $\hat{f}_0, \cdots, \hat{f}_{n-1}$ are n Fourier coefficients and can be obtained by `fft`. For the interpolation $\phi(x)$, we differentiate the form (5),

$$\begin{aligned}
\phi'(x) &= \left(\hat{f}_0 + \sum_{0<k<\frac{n}{2}} \left(\hat{f}_k e^{ikx} + \hat{f}_{n-k} e^{-ikx} \right) + \hat{f}_{n/2} \cos(\frac{nx}{2}) \right)' \\
&= \sum_{0<k<\frac{n}{2}} \left(\hat{f}_k e^{ikx} \cdot ik + \hat{f}_{n-k} e^{-ikx} \cdot (-ik) \right) - \hat{f}_{n/2} \sin(\frac{nx}{2}) \cdot \frac{n}{2} \\
&= \sum_{0<k<\frac{n}{2}} \left(\hat{f}_k e^{ikx} \cdot ik + \hat{f}_{n-k} e^{-ikx} \cdot (-ik) \right) + \hat{f}_{n/2} \frac{1}{2} \left(e^{i\frac{n}{2}x} \cdot i\frac{n}{2} + e^{i(-\frac{n}{2})x} \cdot (-i\frac{n}{2}) \right),
\end{aligned} \tag{6}$$

which is very similar to our implementation of Fourier interpolation, just needs vector multiplication before doing the inverse Fourier transform.

The routine of approximating derivatives on a finer grid (upsampled) for an **even grid** is:

1. Use `fft` on the n interpolation points to obtain Fourier coefficients $\hat{f}_0, \cdots, \hat{f}_{n-1}$;
2. Multiply the Fourier coefficients with the corresponding frequency (we do **not** zero out the special mode, but we would do this if $N = n$!)

$$\hat{\phi}'_k = \hat{f}_k \left(\frac{2\pi}{L} \right) \begin{cases} ik, & k \le n/2, \\ -i(n-k), & k > n/2; \end{cases}$$

3. Apply oversampling to N Fourier coefficients
   $(\hat{c}_k)_{k=1}^N = (\hat{\phi}'_0, \hat{\phi}'_1, \cdots, \hat{\phi}'_{n/2-1}, \frac{\hat{\phi}'_{n/2}}{2}, 0, \cdots, 0, -\frac{\hat{\phi}'_{n/2}}{2}, \hat{\phi}'_{n/2+1}, \cdots, \hat{\phi}'_{n-1})$;
4. Apply `ifft` to $(\hat{c}_k)_{k=1}^N$, obtain the derivative of interpolation estimated on fine grids.

Since we still use `fft, ifft`, just add an vector multiplication, so our cost is still $O(N \log(N))$.

1.3 KdV Equation

We now want to discretize in space:

$$\partial_t \phi = \mathcal{K}\left[\phi(\cdot,t)\right] = -\partial_{xxx}\phi - 3\partial_x\left(\phi^2\right),$$

where $\mathcal{K}\left[\phi(\cdot,t)\right]$ denotes the functional on the right hand side, which only involves derivatives of x. The r.h.s of the KdV equation in Fourier space as

$$\widehat{\mathcal{K}\left[\phi(\cdot)\right]} = \boldsymbol{\mathcal{F}}\left(\mathcal{K}\left[\phi(\cdot)\right]\right) = \boldsymbol{F}\left(\hat{\boldsymbol{\phi}}\right) = ik^3 \boxdot \hat{\boldsymbol{\phi}} - 3i\boldsymbol{k} \boxdot \hat{\boldsymbol{w}},$$

where

$$\hat{\boldsymbol{w}} = \boldsymbol{\mathcal{F}}\left(\left(\boldsymbol{\mathcal{F}}^{-1}\hat{\boldsymbol{\phi}}\right)^{\boxed{2}}\right).$$

Here N is number of nodes for Fourier approximation, and $M > N$ is number of fine nodes.

To compute $\mathcal{K}\left[\phi(\cdot,t)\right]$ when we are given either only $\hat{\boldsymbol{\phi}}$ or both $\hat{\boldsymbol{\phi}}$ and $\boldsymbol{\phi}$ (code design to think about) for even-sized grids:

1. Set a larger size $N' = 2N($ or more efficient but also works $N' = 3N/2)$ if anti-aliasing, or $N' = N$ if not, and conduct the following step:

$$\hat{\boldsymbol{w}} = \text{truncate}\left[\mathcal{F}\left(\left(\mathcal{F}^{-1}(\text{zero-pad}(\hat{\boldsymbol{\phi}}))\right)^{\boxed{2}}\right)\right]. \tag{7}$$

   where **zero-pad** is pad the N Fourier modes to N' and **truncate** is truncate to save only the first N Fourier modes. *What do you do with the unmatched Fourier mode when you truncate?*

2. Multiply the Fourier coefficients with the corresponding frequency to obtain $\widehat{\mathcal{K}\left[\phi(\cdot)\right]}$ (note that again we do **not** zero out the $N/2$ mode unless $M = N$)

$$F_k = \begin{cases} i(\frac{2\pi}{L}k)^3\hat{\phi}_k - 3i\frac{2\pi}{L}k\hat{\phi^2}_k, & k \le N/2, \\ i(-\frac{2\pi}{L}(N-k))^3\hat{\phi}_k - 3i\frac{2\pi}{L}(N-k)\hat{w}_k, & k > N/2, \end{cases}$$

3. Apply oversampling to M points:
   $(\hat{c}_k)_{k=1}^N = (F_0, F_1, \cdots, F_{N/2-1}, \frac{F_{N/2}}{2}, \cdots, -\frac{F_{N/2}}{2}, F_{N/2+1}, \cdots, F_{N-1});$
4. Apply `ifft` to $(\hat{c}_k)_{k=1}^N$, obtain the approximation $\mathcal{K}\left[\phi(\cdot,t)\right]$ estimated on fine grids.