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Numerical Methods for Differential Equations in Physics

Spatial Discretization

Difference with temporal discretization:

find all values $f(x_0), f(x_1), \ldots f(x_N)$ simultaneously

Methods

✓ **Finite Differences**

Finite Volumes

Finite Elements

Spectral $\Longrightarrow$
- ✓ **Pseudospectral**
- **Spectral Elements**

Finite Differences

First derivative

Centered

$$\frac{du}{dx} \approx \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x}$$

Right

$$\frac{du}{dx} \approx \frac{u(x+\Delta x) - u(x)}{\Delta x}$$

Left

$$\frac{du}{dx} \approx \frac{u(x) - u(x-\Delta x)}{\Delta x}$$

General three point formula:

$$\frac{du}{dx} \approx au(x+\Delta x) + bu(x) + cu(x-\Delta x)$$

Taylor series:

$$u(x+\Delta x) = u(x) + \Delta x u'(x) + \frac{\Delta x^2}{2}u''(x) + \frac{\Delta x^3}{6}u'''(x) + \frac{\Delta x^4}{24}u''''$$

$$u(x) = u(x)$$

$$u(x-\Delta x) = u(x) - \Delta x u'(x) + \frac{\Delta x^2}{2}u''(x) - \frac{\Delta x^3}{6}u'''(x) + \frac{\Delta x^4}{24}u''''$$

$$\textbf{Sum} = (a+b+c)u + (a-c)\Delta x u' + (a+c)\frac{\Delta x^2}{2}u'' + (a-c)\frac{\Delta x^3}{6}u'''$$

Term in u''	$0 = a + c$	$\Longrightarrow c = -a$
Term in u	$0 = a + b + c$	$\Longrightarrow b = 0$
Term in u'	$1 = \Delta x(a - c)$	$\Longrightarrow a = -c = 1/(2\Delta x)$
Term in u'''	$(a - c)u'''\Delta x^3/6$	$\Longrightarrow$ **Error** $= u'''\Delta x^2/6$

Centered difference formula is second-order accurate

Second derivative:

$$\textbf{Sum} = (a+b+c)u + (a-c)\Delta x u' + (a+c)\frac{\Delta x^2}{2}u'' + (a-c)\frac{\Delta x^3}{6}u'''$$

Term in u'	$0 = (a-c)$	$\Longrightarrow c = a$
Term in u''	$1 = (a+c)\Delta x^2/2$	$\Longrightarrow a = 1/\Delta x^2$
Term in u	$0 = a+b+c$	$\Longrightarrow b = -2/\Delta x^2$
Term in u'''	$0 = (a-c)$	
Term in u''''	$(a+c)u''''\Delta x^4/24$	$\Longrightarrow$ **Error** $= u''''\Delta x^2/12$

$$\frac{d^2u}{dx^2} = \frac{u(x+\Delta x) - 2u(x) + u(x-dx)}{\Delta x^2} + O(\Delta x^2)$$

Spectral Methods: Differentiation

$$f(x) = \sum_k f_k \, \phi_k(x)$$

$$f'(x) = \sum_k f_k \, \phi'_k(x) = \sum_k f_k \sum_\ell D_{\ell,k} \, \phi_\ell(x)$$
$$= \sum_\ell \left(\sum_k D_{\ell,k} f_k \right) \phi_\ell(x) = \sum_\ell (Df)_\ell \, \phi_\ell(x)$$

Choice of basis functions ϕ depends on boundary conditions.

Periodic boundary conditions over $[0, 2\pi)$ $\Longrightarrow$ truncated Fourier series

$$u(x) = \sum_{k=-N/2+1}^{N/2} \hat{u}_k e^{ikx} \qquad\qquad u \text{ real } \Longrightarrow \hat{u}_{-k} = \hat{u}_k^*$$

Derivatives become multiplications:

$$u'(x) = \sum_k ik\hat{u}_k e^{ikx} \qquad\qquad u''(x) = -\sum_k k^2 \hat{u}_k e^{ikx}$$

In terms of trigonometric functions: N **values** $\{u(x_j), x_j \equiv 2\pi j/N\}$**.**

$$\textbf{For} \begin{cases} k = 0 & \sin(kx) = 0 \\ k = N/2 & \sin(kx_j) = \sin\left(\frac{N}{2}\frac{2\pi j}{N}\right) = \sin(\pi j) = 0 \end{cases}$$

$$\textbf{For} \begin{cases} k = 0 & \cos(kx) = 1 \\ k = N/2 & \cos(kx_j) = \cos\left(\frac{N}{2}\frac{2\pi j}{N}\right) = \cos(\pi j) = (-1)^j \end{cases}$$

$\frac{N}{2} - 1$ **sine coefficients** s_k, $\frac{N}{2} + 1$ **cosine coefficients** c_k, **total =** N**.**

Differentiation from function values ("physical space")

$$\{u(x_j)\} \underset{\text{FFT}}{\Longrightarrow} \{\hat{u}_k\} \underset{\text{mult}}{\Longrightarrow} \{\widehat{Du}_k = ik\hat{u}_k\} \underset{\text{IFFT}}{\Longrightarrow} \{(Du)(x_j)\}$$

Operation count: $O(N \log N)$ **due to FFTs**

Convergence of Fourier series as $N \to \infty$

Interval is $0 \leq x \leq L = 2\pi$ **(for simplicity).**

$$u(x) = \sum_k \hat{u}_k e^{ikx}$$

$$\int_0^{2\pi} dx\, u(x) e^{ik'x} = \sum_k \hat{u}_k \int_0^{2\pi} dx\, e^{ikx} e^{ik'x} = \sum_k \hat{u}_k \delta_{k,k'} 2\pi = 2\pi \hat{u}_{k'}$$

Integration by parts (for $k \neq 0$**)**

$$u = u(x) \qquad du = u'(x)dx$$

$$dv = e^{ikx} dx \qquad v = \frac{1}{ik} e^{ikx}$$

$$2\pi \hat{u}_k = \int_0^{2\pi} dx\, u(x) e^{ikx} = \left[u(x) \frac{1}{ik} e^{ikx} \right]_0^{2\pi} - \int_0^{2\pi} dx \frac{1}{ik} e^{ikx} u'(x) dx$$

If $u(2\pi) = u(0)$ then surface term vanishes:

$$2\pi \hat{u}_k = -\frac{1}{ik} \int_0^{2\pi} dx\, e^{ikx} u'(x)$$ **Integrate by parts again:**

$$= -\frac{1}{ik} \left(\left[u'(x) \frac{1}{ik} e^{ikx} \right]_0^{2\pi} - \int_0^{2\pi} dx \frac{1}{ik} e^{ikx} u''(x) dx \right)$$

If $u'(2\pi) = u'(0)$ then surface term vanishes:

$$2\pi \hat{u}_k = -\frac{1}{k^2} \int_0^{2\pi} dx\, e^{ikx} u''(x)$$ **Integrate by parts again:**

$$= -\frac{1}{k^2} \left(\left[u''(x) \frac{1}{ik} e^{ikx} \right]_0^{2\pi} - \int_0^{2\pi} dx \frac{1}{ik} e^{ikx} u'''(x) dx \right)$$

If $u''(2\pi) = u''(0)$ then surface term vanishes:

$$2\pi \hat{u}_k = -\frac{1}{ik^3} \int_0^{2\pi} dx\, e^{ikx} u'''(x)$$ **Etc.**

If $u^{(p)}(x)$ is periodic and continuous for all p, then

convergence of Fourier coefficients $\hat{u}_k$ is faster than $\frac{1}{k^p}$ for <u>any</u> power p.

Error from truncating series at $|k| \leq \frac{N}{2}$ is less than $O\left(\frac{1}{N^p}\right)$ for <u>any</u> p.

This is called exponential convergence.

Much faster convergence than finite differences:

Largest wavenumber $\frac{N}{2} \Longleftrightarrow$ Smallest wavelength $\lambda = \frac{4\pi}{N}$

Need at least 4 points per wavelength $\Longrightarrow \Delta x = \frac{\lambda}{4} = \frac{\pi}{N}$

Error for p-th order finite difference scheme is

$$(\Delta x)^p \sim \left(\frac{\pi}{N}\right)^p \sim O\left(\frac{1}{N^p}\right)$$

More about accuracy: eigenvalue problem

$\dfrac{d^2u}{dx^2} = \lambda u$ **with periodic boundary conditions over** $[0, 2\pi]$

Eigenfunctions are $\sin kx$, $\cos kx$ **and eigenvalues are** $-k^2$

Act with the second-order finite-difference operator on $\sin kx$**:**

$$
\begin{aligned}
&\frac{1}{\Delta x^2}\left(\sin(k(x+\Delta x)) - 2\sin(kx) + \sin(k(x-\Delta x))\right)\\
=&\frac{1}{\Delta x^2}\left[\sin(kx)\cos(k\Delta x) + \sin(k\Delta x)\cos(kx) - 2\sin(kx)\right.\\
&\quad\left.+\sin(kx)\cos(k\Delta x) - \sin(k\Delta x)\cos(kx)\right]\\
=&\frac{1}{\Delta x^2}\left[\sin(kx)\cos(k\Delta x) - 2\sin(kx) + \sin(kx)\cos(k\Delta x)\right]\\
=&\frac{2}{\Delta x^2}\left[\cos(k\Delta x) - 1\right]\sin(kx)
\end{aligned}
$$

Thus, $\sin(kx)$ **is an eigenvector of the finite-difference second derivative,**

but with eigenvalue

$$\begin{aligned}
\frac{2}{\Delta x^2}\left[\cos(k\Delta x) - 1\right] &= \frac{2}{\Delta x^2}\left[1 - \frac{(k\Delta x)^2}{2} + \frac{(k\Delta x)^4}{24} + \ldots - 1\right] \\
&= \frac{2}{\Delta x^2}\left[-\frac{(k\Delta x)^2}{2} + \frac{(k\Delta x)^4}{24} + \ldots\right] \\
&= -k^2\left[1 - \frac{(k\Delta x)^2}{12} + \ldots\right]
\end{aligned}$$

Spectral Methods: Multiplication

$$u(x) = \sum_{k=-N/2+1}^{N/2} \hat{u}_k e^{ikx} \qquad v(x) = \sum_{\ell=-N/2+1}^{N/2} \hat{v}_\ell e^{i\ell x}$$

$$\begin{aligned} w(x) = (uv)(x) &= \sum_{k=-N/2+1}^{N/2} \hat{u}_k e^{ikx} \sum_{\ell=-N/2+1}^{N/2} \hat{v}_\ell e^{i\ell x} \\ &= \sum_{k=-N/2+1}^{N/2} \sum_{\ell=-N/2+1}^{N/2} e^{i(k+\ell)x} \hat{u}_k \hat{v}_\ell \\ &= \sum_{m=-N+1}^{N} e^{imx} \sum_{k=-N/2+|m|}^{N/2-|m|} \hat{u}_k \hat{v}_{m-k} = \sum_{m=-N+1}^{N} e^{imx} \hat{w}_m \end{aligned}$$

Convolution: takes time $O(N^2)$.

In two dimensions (x, y), takes time $O(N_x^2 N_y^2)$.

Pseudo-spectral method

Derivatives carried out in spectral space

$$f(x) = \sum_k f_k \phi_k(x) \Longrightarrow f'(x) = \sum_k (Df)_k \phi_k(x) \qquad \text{Cost } O(N)$$

Multiplications carried out in physical space

$$(fg)(x_j) = f(x_j)g(x_j) \qquad \text{Cost } O(N)$$

FFTs to go between spectral and physical representations **Cost** $O(N \log N)$

$$\{u(x_j)v(x_j), j = 0, \ldots N-1\} \Longrightarrow \{\widehat{(uv)}_k, -N/2+1 \le k \le N/2\}$$

In two dimensions (x, y)**, costs are** $O(N_x N_y)$ **and** $O(N_x N_y \log(N_x N_y))$

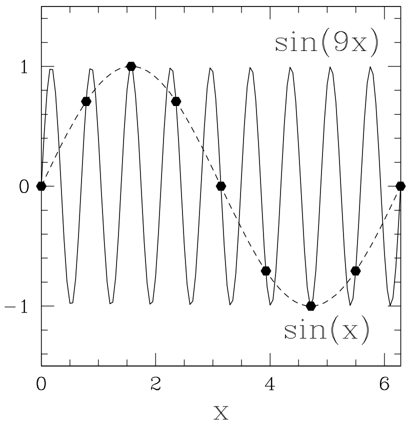
Aliasing

$$u(x) = \sum_{k=-N/2+1}^{N/2} \hat{u}_k e^{ikx} \quad v(x) = \sum_{\ell=-N/2+1}^{N/2} \hat{v}_\ell e^{i\ell x}$$

Exact product $w(x) \equiv (uv)(x) = \sum_{k=-N+1}^{N} \hat{w}_k e^{ikx} \quad k \in [-N, N]$

Aliasing when transform using N instead of $2N$ function values:

$$\{u(x_j)v(x_j), j = 0, \ldots N-1\} \Longrightarrow \{\widehat{(uv)}_k, -N/2+1 \leq k \leq N/2\}$$

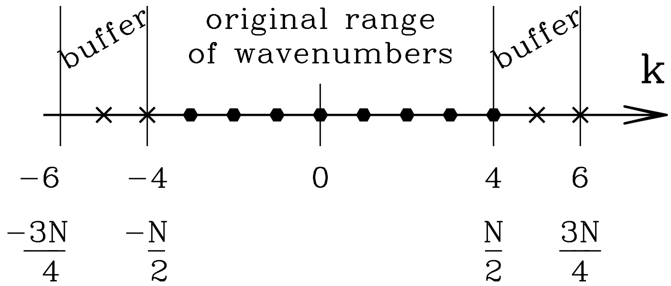


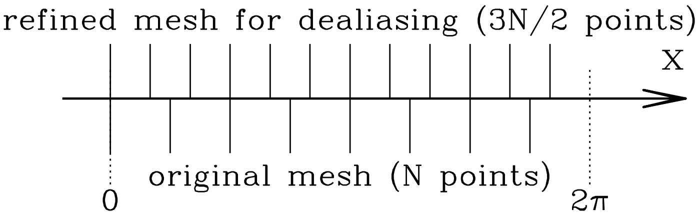
We accept that we cannot represent wavenumbers k with $|k| > N/2$.

But high-wavenumber components are not set to zero: they are misinterpreted as low-wavenumber components!

Sampling at $x_j = 2\pi j/8$,
$\sin(9x)$ is misinterpreted as $\sin(x)$.

De-aliasing





$\{\hat{u}_k, \hat{v}_k, |k| \leq N/2\}$

$\Downarrow$ **pad buffer with zeros**

$\{\hat{u}_k, \hat{v}_k, |k| \leq 3N/4\}$

$\Downarrow$ **IFFT**

$\{u(x_j), v(x_j), j \in [0, 3N/2]\}$

$\Downarrow$ **pointwise multiplication**

$\{w(x_j) = u(x_j)v(x_j), j \in [0, 3N/2]\}$

$\Downarrow$ **FFT**

$\{\hat{w}_k, |k| \leq 3N/4\}$

$\Downarrow$ **truncate to original resolution**

$\{\hat{w}_k, |k| \leq N/2\}$

De-aliasing is often not necessary since for high k, $\hat{u}_k$ (which would be mis-interpreted as low k) has small magnitude due to spectral convergence.

When not to use Fourier series?

If $u^{(n)}$ is not periodic (or, if forced to be periodic, is discontinuous), then decay of $\hat{u}_k$ with k is like $O(1/k^n)$.

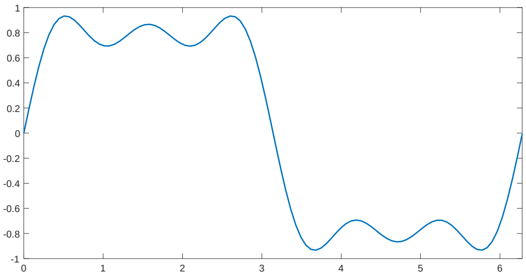
Example: Square wave

$$
\begin{aligned}
f(x) &= \begin{cases} \pi/4 & \text{for } 0 \le x \le \pi \\ -\pi/4 & \text{for } \pi \le x \le 2\pi \end{cases} \\
&= \sin(x) + \frac{1}{3}\sin(3x) + \frac{1}{5}\sin(5x) + \ldots
\end{aligned}
$$

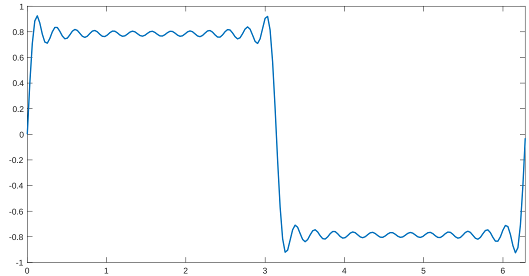
f is discontinuous and so coefficients $\hat{f}_k$ decay like $1/k$ (not very fast).

Gibb's phenomenon

Square-wave Fourier series:



$$\sum_{\substack{j=1\\ j\,\mathrm{odd}}}^{5} \frac{\sin(jx)}{j}$$



$$\sum_{\substack{j=1\\ j\,\mathrm{odd}}}^{25} \frac{\sin(jx)}{j}$$

Although $$\lim_{n\to\infty} \int_{x=0}^{2\pi} dx \left| \sum_{\substack{j=1\\ j\,\mathrm{odd}}}^{n} \frac{\sin(jx)}{j} - f(x) \right|^2 = 0$$

we also have $$\lim_{n\to\infty} \max_{0\le x\le 2\pi} \left| \sum_{\substack{j=1\\ j\,\mathrm{odd}}}^{n} \frac{\sin(jx)}{j} - f(x) \right| \approx 0.18 \times \frac{\pi}{4} \neq 0$$

Non-periodic problems/functions $\Longrightarrow$ use polynomials

(e.g. Dirichlet boundary conditions)

Lagrange polynomials: formalism for interpolation through $\{x_0, x_1, \ldots x_N\}$:

$$\ell_k(x) \equiv \prod_{\substack{j=0 \\ j\neq k}}^{N} \frac{x - x_j}{x_k - x_j}$$

$$\ell_k(x_j) = \delta_{j,k}$$

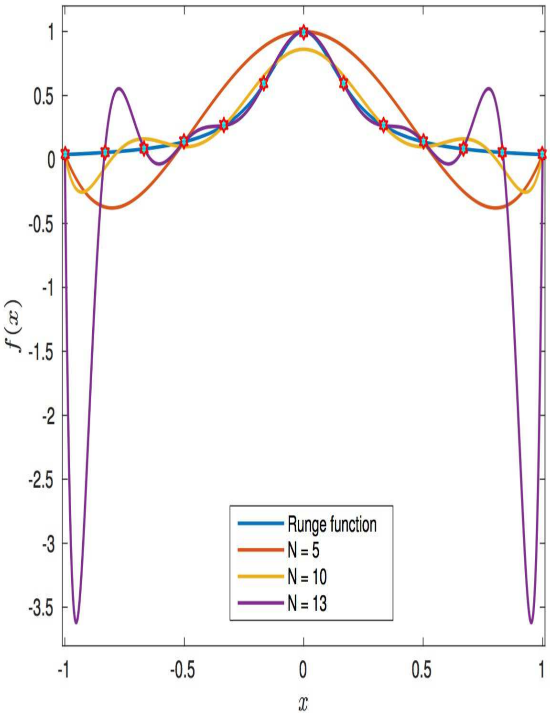
Interpolating polynomial:

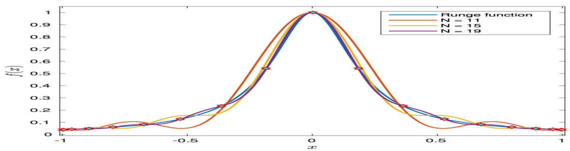
$$P(x) \equiv \sum_{k=0}^{N} f(x_k)\ell_k(x)$$

$$P(x_j) = \sum_{k=0}^{N} f(x_k)\delta_{j,k} = f(x_j)$$

Runge phenomenon. Example of $f(x) = 1/(1+25x^2)$

Equi-spaced points, $N = 5, 10, 13$ **Chebyshev points, $N = 11, 15, 19$**





Sample f at $n+1$ equally spaced points $x_0, x_1, \ldots x_n$ and interpolate n^{th}-order polynomial through $(x_j, f(x_j)) \implies$ oscillations of increasing amplitude as n increases

$$\lim_{n\to\infty} \max_{-1\le x\le 1} \left| \sum_{j=0}^{n} f(x_j)\ell_j(x) - f(x) \right| = \infty$$

Should cluster points at boundaries

Physical reason: boundary layers

Mathematical reason: equispaced points lead to Runge phenomenon

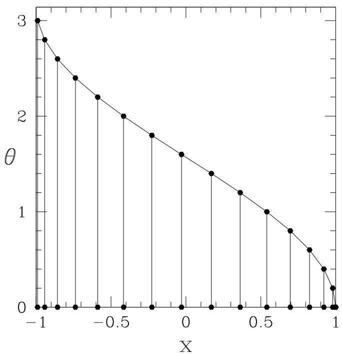
Chebyshev points and Chebyshev functions

$$-1 \le x \le 1 \qquad\qquad 0 \le \theta \le \pi$$

$$x_j = \cos\theta_j \qquad\qquad \theta_j = \frac{\pi j}{N}, \qquad j = 0, \ldots N$$

$$T_n(x) = \cos(n\cos^{-1}(x)) \qquad\qquad T_n(\cos\theta) = \cos(n\theta)$$

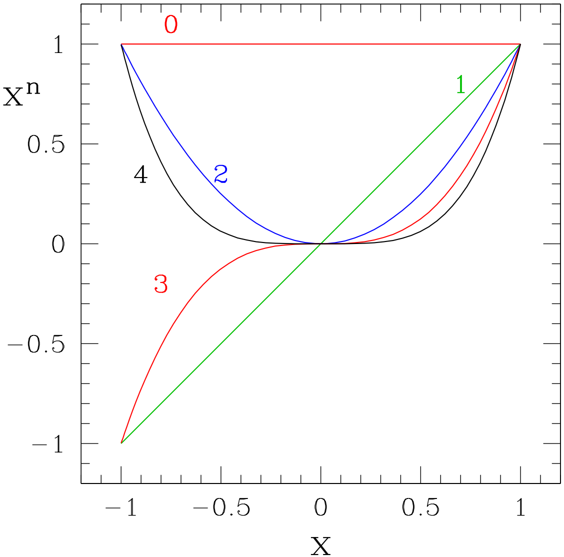
Chebyshev points are clustered at boundaries:



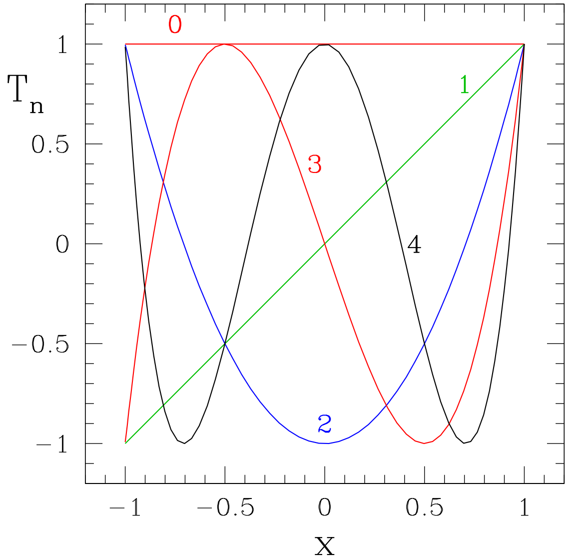
$$x_{j+1} - x_j \sim \Delta\theta \left.\frac{dx}{d\theta}\right|_{\theta_j} = -\frac{\pi}{N}\sin\theta_j$$

$$= -\frac{\pi}{N}\left\{ \begin{array}{ll} \pi/N & \text{for } \theta = \pi/N \\ 1 & \text{for } \theta = \pi/2 \end{array} \right\} = -\left\{ \begin{array}{l} (\pi/N)^2 \\ (\pi/N) \end{array} \right.$$

$x_{j+1} - x_j = 2/N$ **for equally spaced grid on** $[-1, 1]$



Monomials increasingly flat except at boundaries



Chebyshev polynomials

Differentiation of Chebyshev series ("in Chebyshev space")

$$u(x) = \sum_{n=0}^{N} \hat{u}_n T_n(x)$$

$$\frac{d^2u}{dx^2} = \sum_{n=0}^{N} \hat{u}_n T_n''(x) = \sum_{m=0}^{N} \hat{v}_m T_m(x)$$

$$= \sum_{m=0}^{N} \left(\sum_{\substack{n=m+2 \\ n+m\,\text{even}}}^{N} \frac{1}{c_m} n(n^2 - m^2) \hat{u}_n \right) T_m \text{ where } c_m = \begin{cases} 2 & m = 0, N \\ 1 & \text{else} \end{cases}$$

$$\hat{v}_m = \sum_{\substack{n=m+2 \\ n+m\,\text{even}}}^{N} \frac{1}{c_m} n(n^2 - m^2) \hat{u}_n \equiv \sum_{n=0}^{N} R_{m,n} \hat{u}_n$$

There exists a banded matrix B with three non-zero diagonals such that BR is diagonal $\iff$ Recursion relation

$$Rf = g$$

$$BRf = Bg$$

$$4m(m^2 - 1) f_m = (m + 1) c_{m-2} g_{m-2} - 2m g_m + (m - 1) g_{m+2}$$

Differentiation of values on Cheb points ("in physical space")

$$u(x_j) = \sum_{n=0}^{N} \hat{u}_n T_n(x_j)$$

$$u(\cos\theta_j) = v(\theta_j) = \sum_{n=0}^{N} \hat{u}_n \cos(n\theta_j)$$

$\{v(\theta_j)\}$ and $\{\hat{u}_n\}$ are related by the cosine transform.

$$\frac{du}{dx} = \frac{d\theta}{dx}\frac{du}{d\theta}$$

$$x = \cos(\theta)$$

$$\frac{dx}{d\theta} = -\sin\theta = -\sqrt{1-\cos^2(\theta)} = -\sqrt{1-x^2}$$

$$\frac{du}{dx} = \frac{-1}{\sqrt{1-x^2}} \sum_{n=0}^{N} \hat{u}_n (-n) \sin(n\theta_j)$$

$$\{u(x_j)\} \Longrightarrow \{\hat{u}_n\}$$ **cosine transform**

$$\{\hat{u}_n\} \Longrightarrow \{-n\hat{u}_n\}$$ **multiplication**

$$\{-n\hat{u}_n\} \Longrightarrow \left\{\frac{du}{d\theta}(x_j)\right\}$$ **inverse sine transform**

$$\left\{\frac{du}{d\theta}(x_j)\right\} \Longrightarrow \left\{\frac{du}{dx}(x_j) = \frac{-1}{\sqrt{1-x_j^2}}\frac{du}{d\theta}(x_j)\right\}$$ **multiplication**

Trigonometric transforms take time $O(N\log N)$

Multiplications take time $O(N)$

Boundary Conditions

$$u'' = g \qquad \textbf{on } [-1, 1]$$

Impose

$$\alpha_-(t)\ u(-1,t) + \beta_-(t)\ \partial_x u(-1,t) = \gamma_-(t)$$
$$\alpha_+(t)\ u(\quad 1,t) + \beta_+(t)\ \partial_x u(\quad 1,t) = \gamma_+(t)$$

Dirichlet: $\beta = 0, \alpha = 1$
Neumann: $\alpha = 0, \beta = 1$

Homogeneous: $\gamma = 0$
Inhomogeneous $\gamma \neq 0$

Equation at boundaries is replaced by boundary condition

Finite-difference second-derivative matrix, Dirichlet BCs:

$$\frac{1}{\Delta x^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & & \ddots & \\ & & & 1 & -2 \end{bmatrix}\begin{pmatrix} u(x_0) \\ u(x_1) \\ u(x_2) \\ \vdots \\ u(x_N) \end{pmatrix} = \begin{pmatrix} g(x_0) \\ g(x_1) \\ g(x_2) \\ \vdots \\ g(x_N) \end{pmatrix}$$

$$\Longrightarrow \frac{1}{\Delta x^2}\left[\begin{array}{ccccc} 1 & & & & \\ \hline 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & & \ddots & \\ \hline & & & & 1 \end{array}\right]\begin{pmatrix} u(x_0) \\ u(x_1) \\ u(x_2) \\ \vdots \\ u(x_N) \end{pmatrix} = \begin{pmatrix} \gamma_- \\ g(x_1) \\ g(x_2) \\ \vdots \\ \gamma_+ \end{pmatrix}$$

Finite-difference second-derivative matrix, periodic BCs, $x_N = x_0$

$$\frac{1}{\Delta x^2}\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & & \ddots & & \\ & & & & 1 & -2 \end{bmatrix}\begin{pmatrix} u(x_1) \\ u(x_2) \\ u(x_3) \\ \vdots \\ u(x_N) \end{pmatrix} = \begin{pmatrix} g(x_1) \\ g(x_2) \\ g(x_3) \\ \vdots \\ g(x_N) \end{pmatrix}$$

$$\Longrightarrow \frac{1}{\Delta x^2}\left[\begin{array}{cccccc} -2 & 1 & & & & 1 \\ \hline 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & & \ddots & & \\ \hline 1 & & & & 1 & -2 \end{array}\right]\begin{pmatrix} u(x_1) \\ u(x_2) \\ u(x_3) \\ \vdots \\ u(x_N) \end{pmatrix} = \begin{pmatrix} g(x_1) \\ g(x_2) \\ g(x_3) \\ \vdots \\ g(x_N) \end{pmatrix}$$

Chebyshev second-derivative matrix in physical space, Dirichlet BCs:

$$\begin{bmatrix} \\ \textbf{Chebyshev second} \\ \textbf{derivative operator} \\ \textbf{in physical space} \\ \\ \end{bmatrix} \begin{pmatrix} u(x_0) \\ u(x_1) \\ u(x_2) \\ \vdots \\ u(x_N) \end{pmatrix} = \begin{pmatrix} g(x_0) \\ g(x_1) \\ g(x_2) \\ \vdots \\ g(x_N) \end{pmatrix}$$

$$\Longrightarrow \begin{bmatrix} 1 & & \\ \hline & \textbf{Chebyshev second} & \\ & \textbf{derivative operator} & \\ & \textbf{in physical space} & \\ \hline & & 1 \end{bmatrix} \begin{pmatrix} u(x_0) \\ u(x_2) \\ u(x_3) \\ \vdots \\ u(x_N) \end{pmatrix} = \begin{pmatrix} \gamma_- \\ g(x_1) \\ g(x_2) \\ \vdots \\ \gamma_+ \end{pmatrix}$$

Rows enforcing differential equation at boundary points are replaced by BCs. Called “collocation”.

Chebyshev second-derivative matrix in spectral space, Dirichlet BCs:

$$\begin{bmatrix} \textbf{Chebyshev second} \\ \textbf{derivative operator} \\ \textbf{in spectral space} \\ \\ \\ \end{bmatrix} \begin{pmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \vdots \\ \hat{u}_{N-1} \\ \hat{u}_N \end{pmatrix} = \begin{pmatrix} \hat{g}_0 \\ \hat{g}_1 \\ \vdots \\ \hat{g}_{N-1} \\ \hat{g}_N \end{pmatrix}$$

$$\Longrightarrow \left[\begin{array}{ccccc} \multicolumn{5}{c}{\textbf{Chebyshev second}} \\ \multicolumn{5}{c}{\textbf{derivative operator}} \\ \multicolumn{5}{c}{\textbf{in spectral space}} \\ \hline 1 & 1 & 1 & \ldots & 1 \\ 1 & -1 & 1 & \ldots & 1 \end{array} \right] \begin{pmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \vdots \\ \hat{u}_{N-1} \\ \hat{u}_N \end{pmatrix} = \begin{pmatrix} \hat{g}_0 \\ \hat{g}_1 \\ \vdots \\ \gamma_+ \\ \gamma_- \end{pmatrix}$$

$$T_n(1) = 1 \qquad T_n(-1) = (-1)^n$$

Rows enforcing differential equation for highest order polynomials are replaced by BCs. Called "tau".

Fourier: periodic boundary conditions incorporated into representation

Chebyshev: can also incorporate homogeneous BCs into representation

$$\phi_n(x) \equiv \begin{cases} T_n(x) - T_0(x) & \text{for } n \text{ even} \\ T_n(x) - T_1(x) & \text{for } n \text{ odd} \end{cases}$$

Rewrite differential operator using new functions:

$$u(x) = \sum_{n=2}^{N} \hat{u}_n \phi_n(x)$$