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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:

$$u' \approx au(x+\Delta x) + bu(x) + cu(x-\Delta x)$$

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: $u'' \approx au(x+\Delta x) + bu(x) + cu(x-\Delta x)$

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

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** $\{u(x_j), x_j \equiv 2\pi j/N\}$**.**

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

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

$\frac{N}{2} - 1$ **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**

Normalization

Discrete FT	Inverse FT
$\hat{u}_k = \frac{1}{N} \sum_{j=-N/2+1}^{N/2} u(x_j) e^{-ikx_j}$	$u(x_j) = \sum_{k=-N/2+1}^{N/2} \hat{u}_k e^{ikx_j}$
$\hat{u}_k(x) = \frac{1}{\sqrt{N}} \sum_{j=-N/2+1}^{N/2} u(x_j) e^{-ikx_j}$	$u(x_j) = \frac{1}{\sqrt{N}} \sum_{k=-N/2+1}^{N/2} \hat{u}_k e^{ikx_j}$
$\hat{u}_k = \sum_{j=-N/2+1}^{N/2} u(x_j) e^{-ikx_j}$	$u(x_j) = \frac{1}{N} \sum_{k=-N/2+1}^{N/2} \hat{u}_k e^{ikx_j}$

where $x_j = 2\pi j/N$.

More generally, $x_j = Lj/N$ **and need factors** $2\pi/L$, $(2\pi/L)^2$ **in derivatives.**

Ordering

$$\hat{u}_{k+N} = \sum u(x_j) e^{-i(k+N)2\pi j/N} = \sum u(x_j) e^{-ik2\pi j/N} e^{-iN2\pi j/N}$$
$$= \sum e^{-ik2\pi j/N} e^{-i2\pi j} = \hat{u}_{k+N} = \sum u(x_j) e^{-ik2\pi j/N} = \hat{u}_k$$

So Fourier coefficients are N-periodic

$$u(x_j) = \sum_{k=-N/2+1}^{N/2} \hat{u}_k e^{ikx_j} = \sum_{k=0}^{N-1} \hat{u}_k e^{ikx_j}$$

Subroutine output:

$$\begin{array}{llllll} \hat{u}_0 & \hat{u}_1 & \ldots & \hat{u}_{N/2} & \hat{u}_{N/2+1} & \ldots \hat{u}_{N-1} \\ \hat{u}_0 & \hat{u}_1 & \ldots & \hat{u}_{N/2} & \hat{u}_{-N/2+1} & \ldots \hat{u}_{-1} \\ \hat{u}_0 & \hat{u}_1 & \ldots & \hat{u}_{N/2} & \hat{u}^*_{N/2-1} & \ldots \hat{u}^*_1 \end{array} \quad \textbf{if real}$$

Will sometimes want to shift and plot output as:

$$\hat{u}_{-N/2+1} \quad \ldots \hat{u}_{-1} \quad \hat{u}_0 \quad \hat{u}_1 \quad \ldots \quad \hat{u}_{N/2}$$

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

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

$$\hat{u}_k = \int_0^{2\pi} u(x) e^{-ikx} dx$$

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

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

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

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

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

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

Integrate by parts again:

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

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

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

Integrate by parts again:

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

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

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

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

$u'' = \lambda u$ **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 $\sin kx$**:**

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

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

but with eigenvalue

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

Spectral Methods: Multiplication

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

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

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 $O(N \log N)$**

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

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

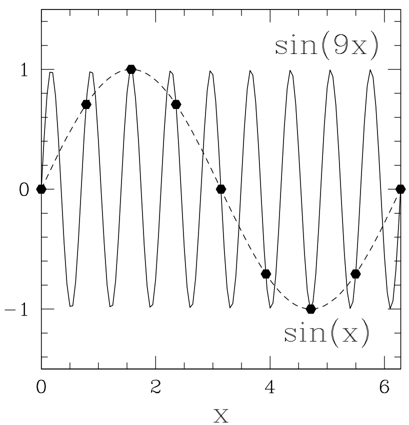
Aliasing

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

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:

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

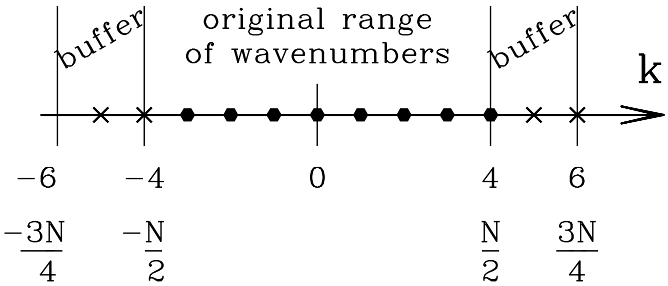


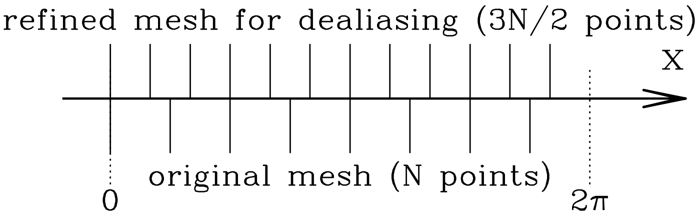
We accept that we cannot represent wavenumbers k with $|k| > N/2$.

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 $O(1/k^n)$.

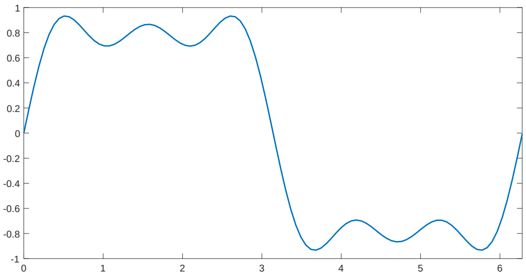
Example: Square wave

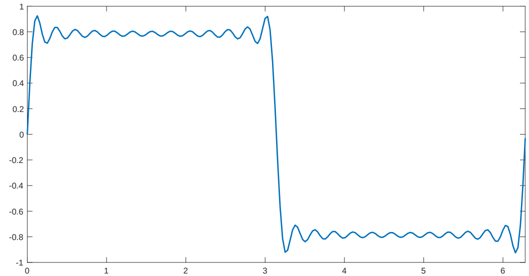
$$f(x) = \begin{cases} \pi/4 & \text{for } 0 \le x \le \pi \\ -\pi/4 & \text{for } \pi \le x \le 2\pi \end{cases}$$
$$= \sin(x) + \frac{1}{3}\sin(3x) + \frac{1}{5}\sin(5x) + \ldots$$

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

Gibb's phenomenon

Square-wave Fourier series:





$$\sum_{\substack{j=1 \\ j \text{odd}}}^{5} \frac{\sin(jx)}{j} \qquad\qquad \sum_{\substack{j=1 \\ j \text{odd}}}^{25} \frac{\sin(jx)}{j}$$

Although

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

we also have

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

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

(e.g. Dirichlet boundary conditions)

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

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

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

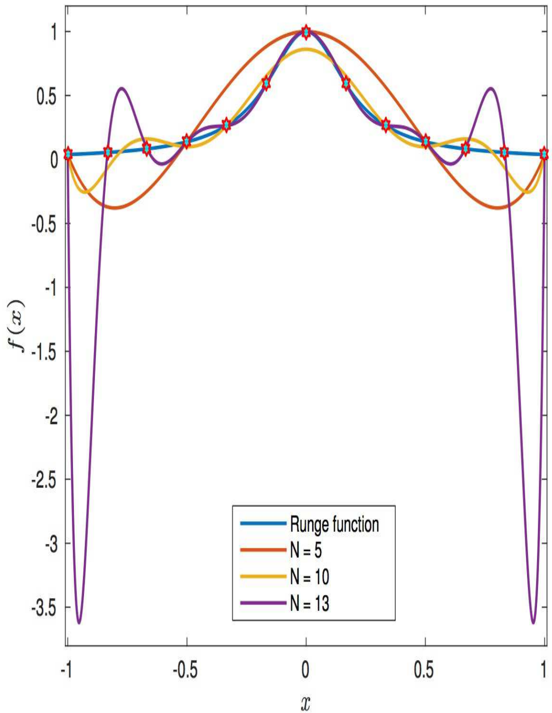
Interpolating polynomial:

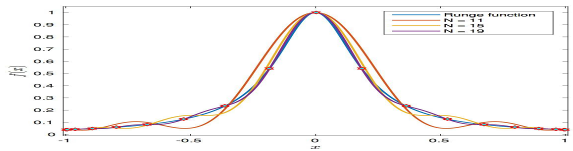
$$P(x) \equiv \sum_{k=0}^{N} f(x_k)\ell_k(x)$$

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

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

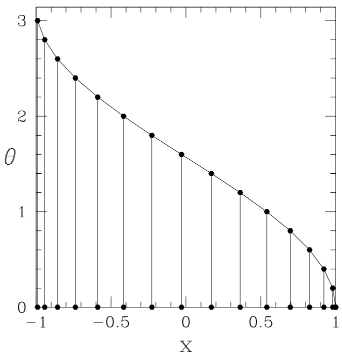
Chebyshev points and Chebyshev functions

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

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

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

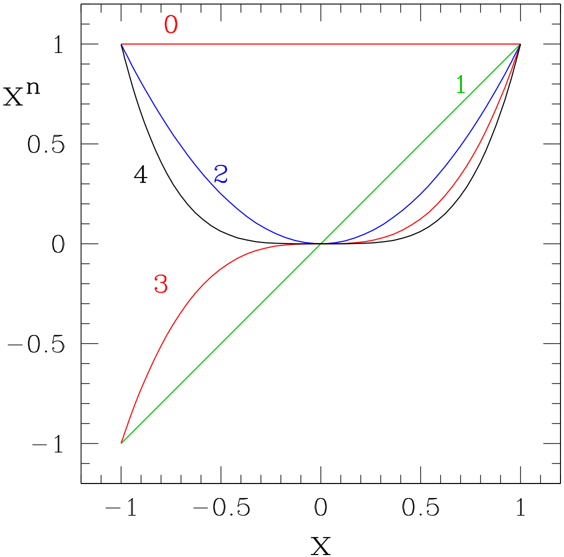
Chebyshev points are clustered at boundaries:



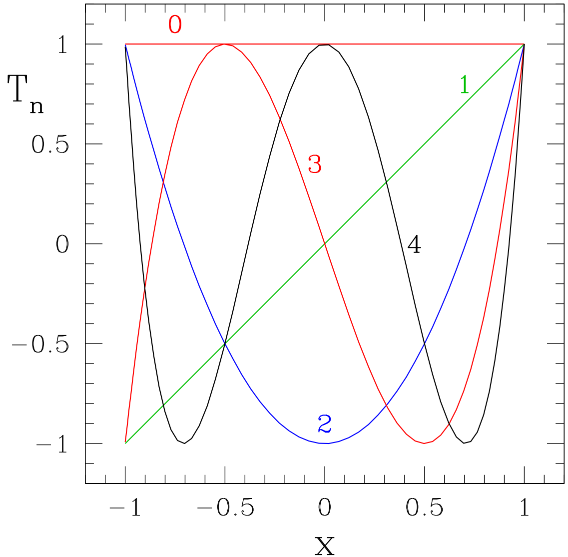
$$x_{j+1} - x_j \sim \Delta\theta \left.\frac{dx}{d\theta}\right|_{\theta_j} = -\frac{\pi}{N}\sin\theta_j$$

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

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



Monomials increasingly flat except at boundaries



Chebyshev polynomials

Differentiation of Chebyshev series ("in Chebyshev space")

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

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

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

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

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

$$Rf = g$$

$$BRf = Bg$$

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

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 $O(N)$

Solving Differential Equations:

Must impose Boundary Conditions

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

Impose

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

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:

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

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

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:

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

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

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".

Permute so that boundary conditions are at top of matrix

(helps with diagonal dominance and use of recursion relation)

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

Fourier: periodic boundary conditions incorporated into representation

Chebyshev: can also incorporate homogeneous BCs into representation

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

Rewrite differential operator using new functions:

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

How to solve linear systems directly?

LU decomposition $\Longleftrightarrow$ Gaussian elimination

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} = \begin{pmatrix} 1 & & & \\ \ell_{21} & 1 & & \\ \ell_{31} & \ell_{32} & 1 & \\ \ell_{41} & \ell_{42} & \ell_{43} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ & u_{22} & u_{23} & u_{24} \\ & & u_{33} & u_{34} \\ & & & u_{44} \end{pmatrix}$$

$$\begin{pmatrix} 1 & & & \\ \ell_{21} & 1 & & \\ \ell_{31} & \ell_{32} & 1 & \\ \ell_{41} & \ell_{42} & \ell_{43} & 1 \end{pmatrix} \underbrace{\left[\begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ & u_{22} & u_{23} & u_{24} \\ & & u_{33} & u_{34} \\ & & & u_{44} \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix} \right]}_{h} = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{pmatrix}$$

$$\begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ & u_{22} & u_{23} & u_{24} \\ & & u_{33} & u_{34} \\ & & & u_{44} \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix} = \begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \end{pmatrix}$$

Find $f_4 = h_4/u_{44}$, then $f_3 = (h_3 - u_{34}f_4)/u_{33}, \ldots$

LU decomposition preserves bandedness

$$\begin{pmatrix} a_{11} & a_{12} & & \\ a_{21} & a_{22} & a_{23} & \\ & a_{32} & a_{33} & a_{34} \\ & & a_{43} & a_{44} \end{pmatrix} = \begin{pmatrix} 1 & & & \\ \ell_{21} & 1 & & \\ & \ell_{32} & 1 & \\ & & \ell_{43} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & & \\ & u_{22} & u_{23} & \\ & & u_{33} & u_{34} \\ & & & u_{44} \end{pmatrix}$$

For $N \times N$ matrix, operation count is $O(N^3)$ for LU decomposition and $O(N^2)$ for backsolve.

For $N \times N$ matrix with J diagonal bands, operation count is $O(J^2N)$ for LU decomposition and $O(JN)$ for backsolve.

LU decomposition is done once, backsolve done for each right-hand-side.

LU preserves bandedness and full rows at bottom or columns on right.

$$
\begin{bmatrix}
\times & \times & & & & & & & & & \times \\
\times & \times & \times & & & & & & & & \times \\
 & \times & \times & \times & & & & & & & \times \\
 & & \times & \times & \times & & & & & & \times \\
 & & & \times & \times & \times & & & & & \times \\
 & & & & \times & \times & \times & & & & \times \\
 & & & & & \times & \times & \times & & & \times \\
 & & & & & & \times & \times & \times & & \times \\
 & & & & & & & \times & \times & \times & \times \\
 & & & & & & & & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times & \times & \times & \times & \times
\end{bmatrix}
=
\begin{bmatrix}
1 & & & & & & & & & & \\
\times & 1 & & & & & & & & & \\
 & \times & 1 & & & & & & & & \\
 & & \times & 1 & & & & & & & \\
 & & & \times & 1 & & & & & & \\
 & & & & \times & 1 & & & & & \\
 & & & & & \times & 1 & & & & \\
 & & & & & & \times & 1 & & & \\
 & & & & & & & \times & 1 & & \\
 & & & & & & & & \times & 1 & \\
\times & \times & \times & \times & \times & \times & \times & \times & \times & \times & 1
\end{bmatrix}
\begin{bmatrix}
\times & \times & & & & & & & & & \times \\
 & \times & \times & & & & & & & & \times \\
 & & \times & \times & & & & & & & \times \\
 & & & \times & \times & & & & & & \times \\
 & & & & \times & \times & & & & & \times \\
 & & & & & \times & \times & & & & \times \\
 & & & & & & \times & \times & & & \times \\
 & & & & & & & \times & \times & & \times \\
 & & & & & & & & \times & \times & \times \\
 & & & & & & & & & \times & \times \\
 & & & & & & & & & & \times
\end{bmatrix}
$$

UL preserves bandedness and full rows at top or columns on left.

$$
\begin{bmatrix}
\times & \times & \times & \times & \times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & & & & & & & & \\
\times & \times & \times & \times & & & & & & & \\
\times & & \times & \times & \times & & & & & & \\
\times & & & \times & \times & \times & & & & & \\
\times & & & & \times & \times & \times & & & & \\
\times & & & & & \times & \times & \times & & & \\
\times & & & & & & \times & \times & \times & & \\
\times & & & & & & & \times & \times & \times & \\
\times & & & & & & & & \times & \times & \times \\
\times & & & & & & & & & \times & \times
\end{bmatrix}
=
\begin{bmatrix}
\times & \times & \times & \times & \times & \times & \times & \times & \times & \times & \times \\
 & \times & \times & & & & & & & & \\
 & & \times & \times & & & & & & & \\
 & & & \times & \times & & & & & & \\
 & & & & \times & \times & & & & & \\
 & & & & & \times & \times & & & & \\
 & & & & & & \times & \times & & & \\
 & & & & & & & \times & \times & & \\
 & & & & & & & & \times & \times & \\
 & & & & & & & & & \times & \times \\
 & & & & & & & & & & \times
\end{bmatrix}
\begin{bmatrix}
1 & & & & & & & & & & \\
\times & 1 & & & & & & & & & \\
\times & \times & 1 & & & & & & & & \\
\times & & \times & 1 & & & & & & & \\
\times & & & \times & 1 & & & & & & \\
\times & & & & \times & 1 & & & & & \\
\times & & & & & \times & 1 & & & & \\
\times & & & & & & \times & 1 & & & \\
\times & & & & & & & \times & 1 & & \\
\times & & & & & & & & \times & 1 & \\
\times & & & & & & & & & \times & 1
\end{bmatrix}
$$

Recall tau method for imposing BCs on $u'' = g$ on $[-1, 1]$ with Cheb poly:

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

Odd and even Cheb polynomials are decoupled.

Can decouple BCs: $u(\pm 1) = \gamma_\pm \Longrightarrow \frac{1}{2}\left(u(1) \pm u(-1)\right) = \frac{1}{2}\left(\gamma_+ \pm \gamma_-\right)$

$$T_n(\pm 1) = (\pm 1)^n \Longrightarrow \frac{1}{2}\left(T_n(1) + T_n(-1)\right) = \frac{1}{2}\left(1 + (-1)^n\right) = \begin{cases} 1 & n \text{ even} \\ 0 & n \text{ odd} \end{cases}$$

$$\Longrightarrow \left[\begin{array}{ccccc} 1 & 0 & 1 & \dots & 1 \\ 0 & 1 & 0 & \dots & 0 \\ \hline \multicolumn{5}{c}{\textbf{Chebyshev second}} \\ \multicolumn{5}{c}{\textbf{derivative operator}} \\ \multicolumn{5}{c}{\textbf{in spectral space}} \end{array}\right] \begin{pmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \vdots \\ \hat{u}_{N-1} \\ \hat{u}_N \end{pmatrix} = \begin{pmatrix} \left(\gamma_+ + \gamma_-\right)/2 \\ \left(\gamma_+ - \gamma_-\right)/2 \\ \hline \hat{g}_0 \\ \hat{g}_1 \\ \vdots \end{pmatrix}$$

Even/odd decoupling: $N \times N$ **matrix** $\Longrightarrow$ **Two** $N/2 \times N/2$ **matrices**
Matrix-vector mult or solve takes time $N^2 \Longrightarrow 2(N/2)^2 = N^2/2$

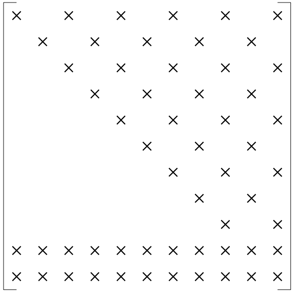
Second-derivative Chebyshev matrix R **is upper triangular.**
There exists a banded matrix B **with three non-zero diagonals such that** BR **is diagonal** $\Longleftrightarrow$ **Recursion relation**

$$
\begin{aligned}
Rf &= g \\
BRf &= Bg \\
4m(m^2-1)f_m &= (m+1)c_{m-2}g_{m-2} - 2mg_m + (m-1)g_{m+2}
\end{aligned}
$$

Matrix-vector mult or solve takes time $[2(N/2)^2] \Longrightarrow [2(N/2)3] = 3N$

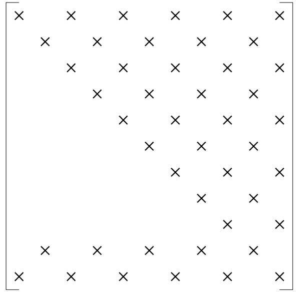
Time for LU decomposition is reduced even more:

$$N^3 \Longrightarrow 2(N/2)^3 \Longrightarrow 2(N/2)3^2 = 9N$$



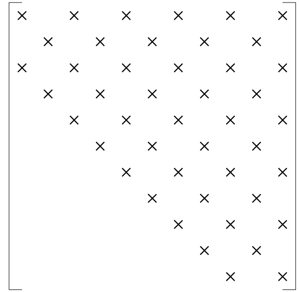
Cheb 2nd deriv

$u(\pm 1) = \gamma_\pm$

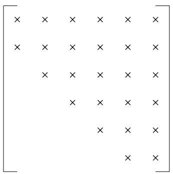


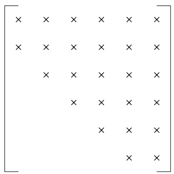
Cheb 2nd deriv

$u(1) \pm u(-1) = \gamma_+ \pm \gamma_-$

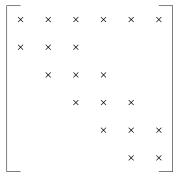


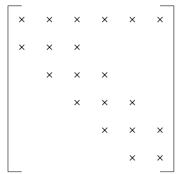
Permute BCs to top





$\rightarrow$ **even** **odd**





$\rightarrow$ **even banded** **odd banded**