Numerical Methods II (Pseudo)Spectral Methods for PDEs

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Convolutions using FFT

Filtering using FFTs

- Because FFT is a very fast, almost linear algorithm, it is used often to accomplish tasks in data processing, e.g., **noise filtering** (see example in previous lecture), computing **(auto)correlation** functions, etc.
- Denote the (continuous or discrete) Fourier transform with

$$\hat{\mathbf{f}} = \mathcal{F}\left(\mathbf{f}
ight)$$
 and $\mathbf{f} = \mathcal{F}^{-1}\left(\hat{\mathbf{f}}
ight)$

- Plain FFT is used in signal processing for digital filtering (low-pass, high-pass, or band-pass filters)
- How to do it: Multiply the spectrum by a filter $\hat{S}(k)$ discretized as $\hat{\mathbf{s}} = \left\{ \hat{S}(k) \right\}_{k}$:

$$\mathbf{f}_{\mathsf{filtered}} = \mathcal{F}^{-1}\left(\hat{\mathbf{s}} \boxdot \hat{\mathbf{f}}
ight) = \mathbf{f} \circledast \mathbf{s},$$

where \boxdot denotes element-wise product, and \circledast denotes convolution.

Convolution

 For continuous function, an important type of operation found in practice is convolution (smoothing) of a (periodic) function f(x) with a (periodic) kernel K(x):

$$(K \circledast f)(x) = \int_0^{2\pi} f(y) K(x-y) dy.$$

• It is not hard to prove the **convolution theorem**:

$$\mathcal{F}(K \circledast f) = \mathcal{F}(K) \boxdot \mathcal{F}(f).$$

• Importantly, this remains true for **discrete convolutions**:

$$(\mathbf{K} \circledast \mathbf{f})_j = rac{1}{N} \sum_{j'=0}^{N-1} f_{j'} K_{j-j'} \quad \Rightarrow$$

 $\mathcal{F}(\mathsf{K} \circledast \mathsf{f}) = \mathcal{F}(\mathsf{K}) \boxdot \mathcal{F}(\mathsf{f}) \quad \Rightarrow \quad \mathsf{K} \circledast \mathsf{f} = \mathcal{F}^{-1}(\mathcal{F}(\mathsf{K}) \boxdot \mathcal{F}(\mathsf{f}))$

Convolutions using FFT

Proof of Discrete Convolution Theorem

Assume that the normalization used is a factor of N^{-1} in the forward and no factor in the inverse DFT:

$$f_{j} = \sum_{k=0}^{N-1} \hat{f}_{k} \exp\left(\frac{2\pi i j k}{N}\right), \text{ and } \hat{f}_{k} = \frac{1}{N} \sum_{j=0}^{N-1} f_{j} \exp\left(-\frac{2\pi i j k}{N}\right)$$
$$\left[\mathcal{F}^{-1}\left(\mathcal{F}\left(\mathsf{K}\right) \boxdot \mathcal{F}\left(\mathsf{f}\right)\right)\right]_{k} = \sum_{k=0}^{N-1} \hat{f}_{k} \hat{K}_{k} \exp\left(\frac{2\pi i j k}{N}\right) =$$
$$^{2} \sum_{k=0}^{N-1} \left(\sum_{l=0}^{N-1} f_{l} \exp\left(-\frac{2\pi i l k}{N}\right)\right) \left(\sum_{m=0}^{N-1} K_{m} \exp\left(-\frac{2\pi i m k}{N}\right)\right) \exp\left(\frac{2\pi i j k}{N}\right)$$
$$= N^{-2} \sum_{l=0}^{N-1} f_{l} \sum_{m=0}^{N-1} K_{m} \sum_{k=0}^{N-1} \exp\left[\frac{2\pi i (j-l-m) k}{N}\right]$$

 N^{-}

contd.

Recall the key discrete orthogonality property

$$\forall \Delta k \in \mathbb{Z} : \quad N^{-1} \sum_{j} \exp\left[i \frac{2\pi}{N} j \Delta k\right] = \delta_{\Delta k} \quad \Rightarrow$$

$$N^{-2} \sum_{l=0}^{N-1} f_l \sum_{m=0}^{N-1} K_m \sum_{k=0}^{N-1} \exp\left[\frac{2\pi i \left(j-l-m\right)k}{N}\right] = N^{-1} \sum_{l=0}^{N-1} f_l \sum_{m=0}^{N-1} K_m \delta_{j-l-m}$$
$$= N^{-1} \sum_{l=0}^{N-1} f_l K_{j-l} = (\mathbf{K} \circledast \mathbf{f})_j$$

Computing convolutions requires 2 forward FFTs, one element-wise product, and one inverse FFT, for a total cost $N \log N$ instead of N^2 . We can use this to solve **periodic integro-differential equations** involving convolutions, for example (recall that trapezoidal rule for the convolution is spectrally accurate for analytic functions)!

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Spectral Differentiation

Spectral Derivative

- Consider approximating the derivative of a periodic function f(x), computed at a set of N equally-spaced nodes, f.
- We can differentiate the spectral approximation: Spectral derivative

$$f'(x) \approx \phi'(x) = \frac{d}{dx}\phi(x) = \frac{d}{dx}\left(\sum_{k=0}^{N-1} \hat{f}_k e^{ikx}\right) = \sum_{k=0}^{N-1} \hat{f}_k \frac{d}{dx}e^{ikx}$$
$$= \sum_{k=0}^{N-1} \left(ik\hat{f}_k\right)e^{ikx} = \sum_{k=0}^{N-1} \left(\widehat{\phi'}\right)_k e^{ikx} \quad \Rightarrow$$
$$\widehat{(\phi')}_k = ik\hat{f}_k \quad \Rightarrow \quad \phi' = \mathcal{F}^{-1}\left(i\mathbf{k} \boxdot \hat{\mathbf{f}}\right)$$

• Differentiation, like convolution, becomes multiplication in Fourier space.

Indeed $-\int f(y)\delta'(x-y)\,dy = \int f'(y)\delta(x-y)\,dy = f'(x).$

Unmatched mode

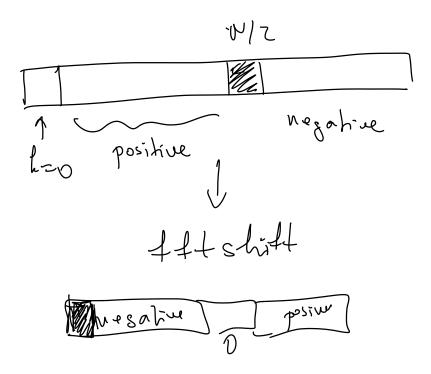
- Recall that for even N there is one unmatched mode, the one with the highest frequency and amplitude $\hat{f}_{N/2}$.
- We need to choose what we want to do with that mode; see notes by S. G. Johnson (MIT) linked on webpage for details:

$$\phi(x) = \hat{f}_0 + \sum_{0 < k < N/2} \left(\hat{f}_k e^{ikx} + \hat{f}_{N-k} e^{-ikx} \right) + \hat{f}_{N/2} \cos\left(\frac{Nx}{2}\right).$$

This is the unique "minimal oscillation" trigonometric interpolant.Differentiating this we get

$$\widehat{(\phi')}_{k} = \widehat{f}_{k} \begin{cases} 0 & \text{if } k = N/2 \\ ik & \text{if } k < N/2 \\ i(k-N) & \text{if } k > N/2 \end{cases}$$

• Real valued interpolation samples result in **real-valued** $\phi(x)$ for all x.



FFT-based differentiation

% From Nick Trefethen's Spectral Methods book
% Differentiation of
$$exp(sin(x))$$
 on $(0,2*pi]$:
N = 8; % Even number!
h = $2*pi/N$; x = $h*(1:N)$ ';
v = $exp(sin(x))$; vprime = $cos(x).*v$;
v_hat = $fft(v)$;
ik = $1i*(0:N/2-1)(0-N/2+1:-1)$ '; % Zero special mode
w_hat = ik .* v_hat;
w = $real(ifft(w_hat))$; Always beh inag is
error = norm(w-vprime, inf)
S with

Differentiation matrices

- Writing g = f' we can denote this in matrix notation $\hat{\mathbf{g}} = \widehat{\mathbf{D}}_1 \hat{\mathbf{f}}$, where $\widehat{\mathbf{D}}_1$ is a **diagonal differentiation matrix** with *ik* on its diagonal (why does it have to be a matrix?).
- Observe that $\widehat{\mathbf{D}}_{1}^{\star} = -\widehat{\mathbf{D}}_{1}$ (anti-Hermitian).
- In real space $\mathbf{g} = \mathbf{D}\mathbf{f}$ and in Fourier space $\hat{\mathbf{g}} = \widehat{\mathbf{D}}\hat{\mathbf{f}}$, related by

$$D = F^{-1}\widehat{D}F = F^{*}\widehat{D}F, \subset an fisyumetric$$

where **F** is the unitary DFT matrix. Observe this is a similarity transformation!

• Here Ff and $F^{\star}\hat{f}$ are computed using the (forward/inverse) FFT in nearly linear time.

Second derivative

• Differentiating the interpolant twice we get

$$\widehat{(\phi'')}_k = \widehat{f}_k \begin{cases} -k^2 & \text{if } k < N/2 \\ -(k-N)^2 & \text{if } k \ge N/2 \end{cases}$$

- Similarly, if g = f'' then $\hat{\mathbf{g}} = \widehat{\mathbf{D}}_2 \hat{\mathbf{f}}$, where $\widehat{\mathbf{D}}_2$ has $-k^2$ on its diagonal, $\widehat{\mathbf{D}}_2^* = \widehat{\mathbf{D}}_2$ (Hermitian, same for \mathbf{D}_2).
- Double differentiating is different from differentiating twice in sequence, i.e., $\mathbf{D}_2 \neq \mathbf{D}_1^2$.
- Why is D_2 "better" than D_1^2 ? They have the same spectral accuracy.
- \mathbf{D}_1^2 has a nontrivial null space of $\mathbf{1}$ and $\mathbf{F}^{-1}\mathbf{e}_{N/2}$, while \mathbf{D}_2 has only $\mathbf{1}$.
- So **D**₂ is closer to the **continuum Laplacian operator** in periodic domains (having only constant functions in its null space). This is important when solving elliptic/parabolic PDEs.

 $\nabla^{Z} \mathcal{U}(\vec{x}) = f(\vec{y})$ $\int_{2} = F^{*} D_{2} F$ $D_z u = f$ $\begin{array}{ccc}
n & n \\
D_{1} & n & -1
\end{array}$ $\hat{\mathcal{X}} = (\hat{\mathcal{D}}_{z})^{-1} \hat{\mathcal{I}}$ 1 1 12

Discrete Matrices vs Continuum Operators

- The lesson learned from $D_2 \neq D_1^2$ is quite general: Continuum identities don't always translate to discrete identities.
- Many properties that seem obvious in continuum, may not work for discretizations:
 - Chain and product rules e.g., (cu)' = c'u + cu'.
 - Integration by parts (including boundary terms).
 - Operators commute, e.g., $\partial_x (\partial_y f) = \partial_y (\partial_x f)$.
 - Null spaces, eigenvalue spectrum properties (e.g., positive definiteness, symmetry, etc.).
- Mimetic discretizations try to mimic some of the properties of continuum operators.



Sturm-Louville Problems

• As an example, consider the periodic Sturm-Louville (SL) operator appearing in many boundary-value problems (BVPs):

$$\mathcal{L} = -\frac{d}{dx}c(x)\frac{d}{dx}, \quad c(x) > 0.$$

- From PDE class we know that this is a symmetric positive semidefinite (SPsD) differential operator with only constant functions in its null space; proving this uses integration by parts.
- When discretized, this will become a matrix **L**. We want this matrix to be SPsD with only **e** in its null space.
- It is a bad idea is to use the chain rule and discretize:

$$-\mathcal{L}f = \frac{d}{dx}c(x)\frac{d}{dx}f(x) = c'f' + cf''$$
$$-\mathbf{L}f = (\mathbf{D}_{1}\mathbf{c}) \boxdot (\mathbf{D}_{1}\mathbf{f}) + c \boxdot (\mathbf{D}_{2}\mathbf{f}) \quad (BAD!)$$
since this is not an SPsD L.

Pseudospectral SL operator

- In words: Go to Fourier space using the FFT, multiply coefficients by *ik*, go back to real space with iFFT, multiply by *c*(*x*) in real-space, then go back to Fourier space (FFT) and multiply coefficients by *-ik*, and then go back to real space again (iFFT).
- Why does this work? In matrix notation

$$\mathbf{L} = -\left(\mathbf{F}^{\star}\widehat{\mathbf{D}}_{1}\mathbf{F}\right)\mathbf{C}\left(\mathbf{F}^{\star}\widehat{\mathbf{D}}_{1}\mathbf{F}\right) = \mathbf{D}_{1}\mathbf{C}\mathbf{D}_{1}^{\star},$$

where **C** is a diagonal matrix with $\mathbf{c} > 0$ on its diagonal. • This is obviously SPsD since **C** is SPD (why?).

Pseudospectral SL algorithm

For even N the pseudo-spectral L has a nontrivial null space just like D_1^2 does (think c = 1), but this can be fixed (see article by Johnson):

- **Or Compute f' using FFT/iFFT** but save the coefficient $\hat{f}_{N/2}$ (two FFTs).
- 2 Compute $\mathbf{g} = \mathbf{c} \boxdot \mathbf{f}'$ in real space (pseudospectral part).
- Ompute ĝ using FFT.
- Compute $(\mathbf{L}\mathbf{f})$ in Fourier space as:

$$\widehat{(\mathbf{Lf})}_{k} = \begin{cases} \widehat{c}_{0} \left(\frac{N}{2}\right)^{2} \widehat{f}_{N/2} & \text{if } k = N/2 \\ -ik\widehat{g}_{k} & \text{if } k < N/2 \\ -i\left(k-N\right)\widehat{g}_{k} & \text{if } k > N/2 \end{cases}$$

Sompute **Lf** in real space using an iFFT.

Solving PDEs using FFTs

Solving PDEs using FFTs

KdV equation

• Consider as an example the periodic Korteweg – de Vries equation on $[0, 2\pi)$,

$$\partial_t \phi = -\partial_{\mathsf{x}\mathsf{x}\mathsf{x}}\phi + \mathbf{6}\phi\left(\partial_{\mathsf{x}}\phi\right),$$

which models waves in a channel and has soliton solutions.

- First note that $\phi \phi_x = \partial_x \left(\phi^2/2 \right)$ and this is the right form to use because **KdV** is a conservation law and $\phi^2/2$ is a flux.
- Not all forms of PDEs equivalent on paper are equivalent numerically! We prefer

$$\partial_t \phi = -\partial_{xxx} \phi + 3\partial_x \left(\phi^2\right).$$

• The idea is to use a Fourier series representation,

$$\phi(x,t) = \sum_{k} \hat{\phi}_{k}(t) e^{ikx}.$$

Spectral spatial discretization

If we go to Fourier space we get a system of coupled (nonlinear)
 ODEs:

$$\begin{array}{c}
\frac{d\hat{\phi}_{k}}{dt} = ik^{3}\hat{\phi}_{k} + 3ik(\widehat{\phi}^{2})_{k} \Rightarrow \varphi_{\text{in real space}} \\
\frac{d\hat{\phi}}{dt} = ik^{3} \odot \hat{\phi} + 3ik \odot \mathcal{F}\left(\left(\mathcal{F}^{-1}\hat{\phi}\right)^{2}\right). \\
\end{array}$$

- Note that the unmatched mode N/2 should be set to zero for the third derivative (all odd derivatives in fact).
- This is a **pseudo-spectral spatial discretization** and will be spectrally accurate for analytic solutions.
- In order to actually compute solutions we need methods to solve systems of ODEs (coming up soon)!

with

Nonlinear PDEs

• Observe that if the nonlinear term was not there, we could write the solution right away: $\psi_{\mathcal{L}} = \psi_{\mathcal{L}} + \psi_{\mathcal{$

$$\hat{\phi}_k(t) = \hat{\phi}_k(0) \exp(ik^3 t)$$
 for all k .

- This is called an **exponential temporal integrator** and can be used to build accurate integrators for the nonlinear KdV equation.
- If the equation were linear, then $\hat{\phi}_k(t) = 0$ if $\hat{\phi}_k(0) = 0$: linear **PDEs do not generate new Fourier components.**
- But this is not true for nonlinear equations: in general, the solution will have nonzero components for all k for sufficiently long times, and aliasing becomes a problem.
- An extreme example is Burger's equation, which develops singularities (shocks), leading to the Gibbs phenomenon and loss of spectral accuracy.

Aliasing

• As an example, consider the product (or square)

 $w(x) = u(x)v(x) \Rightarrow$

$$w(x) = \left(\sum_{k''=-n}^{n} \hat{u}_{k''} e^{ik''x}\right) \left(\sum_{k=-n}^{n} \hat{u}_{k'} e^{ik'x}\right) = \sum_{k=-2n}^{2n} \hat{w}_k e^{ikx}$$

- So we doubled the number of Fourier modes, and handling this would require growing our FFT grid along the way!
- What we want to compute is the truncated Fourier series

$$w(x) \approx \tilde{w}(x) = \sum_{k=-n}^{n} \hat{w}_k e^{ikx}.$$

 If we do this naively using FFTs on a grid of N = 2n + 1 points, however, we will alias the modes |k| > n with those with |k| < n and this will introduce aliasing error.

C(x) = n

Anti-aliasing via oversampling

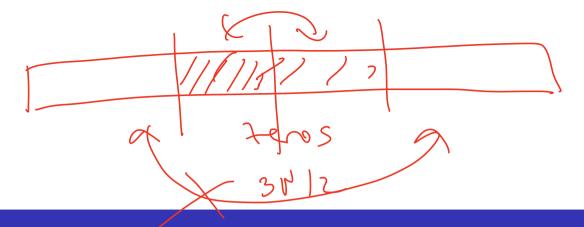
- But there is an easy fix using **oversampling**. Take u = v for simplicity and even N: M = 3N(2 is Minute L)
- **1** Evaluate u(x) on a grid of N points, take the FFT to compute $\hat{\mathbf{u}}$.
- **2** Padd the FFT to size M = 2N, avoiding fftshift (see fftinterp):

 $(\hat{\mathbf{u}})_{\text{padded}} = \begin{bmatrix} \hat{\mathbf{u}} (1 : N/2) & \text{zeros}(1, M - N) & \hat{\mathbf{u}} (N/2 + 1 : \text{end}) \end{bmatrix}.$

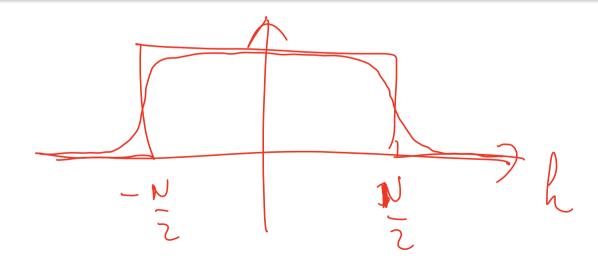
Note: It can be shown that M = 3N/2 also gives the same result.

- 3 Compute an oversampled $u_{os}(x)$ on a grid of size 2N by taking the iFFT of $(\hat{\mathbf{u}})_{padded}$.
- Ocompute \mathbf{u}_{os}^{2} in real space, and take the FFT to compute $\hat{\mathbf{w}}$.
- Solution Truncate to N Fourier coefficients by returning $[\hat{\mathbf{w}}(1:N/2) \quad \hat{\mathbf{w}}(M-N/2+1:end)].$

Chebyshev Series via FFTs



Chebyshev Series via FFTs



Chebyshev Polynomials

- If we are solving PDEs on a bounded interval, say [−1, 1] for simplicity, we need other orthogonal polynomials, not trig ones.
- Recall from Numerical Methods I the Chebyshev polynomials:

 $T_n(x \in [-1,1]) = \cos(n\theta)$ where $x = \cos(\theta \in [0,2\pi])$.

$$T_0(x) = 1$$
, $T_1(x) = x$, $T_2(x) = 2x^2 - 1$, $T_3(x) = 4x^3 - 3x$,...

• These are orthogonal with respect to the weighted inner/dot product:

$$\int_{-1}^{1} T_m(x) T_n(x) \frac{dx}{\sqrt{1-x^2}} = \begin{cases} \pi & m=n=0\\ \pi/2 & m=n>0\\ 0 & m\neq n \end{cases}$$

Chebyshev Series via FFTs

Chebyshev Interpolants

We can represent functions using these polynomials as basis functions,

$$f(x) = \sum_{n=0}^{\infty} \check{f}_n T_n(x) \Rightarrow$$
$$\check{f}_{n>0} = \frac{2}{\pi} \int_{-1}^{1} f(x) T_n(x) \frac{dx}{\sqrt{1-x^2}}$$

• We discretize the function pointwise at N + 1 Chebyshev nodes

$$egin{aligned} & heta_j = j\pi/N, \quad j = 0 \dots N \ & heta_j = \cos heta_j \end{aligned}$$

• This gives us the **Chebyshev interpolant** (approximation):

$$\phi(x) = \sum_{n=0}^{N} \breve{f}_n T_n(x).$$

Chebyshev Nodes

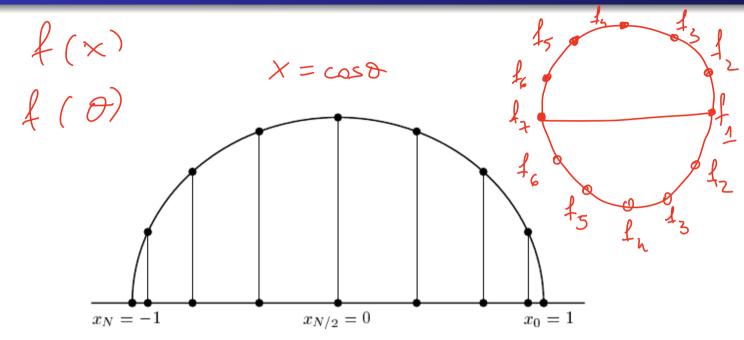


Fig. 5.1. Chebyshev points are the projections onto the x-axis of equally spaced points on the unit circle. Note that they are numbered from right to left.

Chebyshev via Fourier

• Changing variables from x to θ we get

$$\begin{split} \breve{f}_{n>0} &= \frac{2}{\pi} \int_{-1}^{1} f(x) T_n(x) \frac{dx}{\sqrt{1-x^2}}. \\ &= \int_{-\pi}^{\pi} f\left(\cos\theta\right) \cos\left(n\theta\right) d\theta \\ &= \int_{-\pi}^{\pi} f\left(\cos\theta\right) \left(\frac{\exp\left(in\theta\right) + \exp\left(-in\theta\right)}{2}\right) d\theta. \end{split}$$

• So if we consider instead of f(x) the function

$$g(\theta) = f(\cos\theta)$$

then we can go from **Fourier coefficients** of g to **Chebyshev** for f:

$$\breve{f}_{n>0} = \hat{g}_{-n} + \hat{g}_n$$

Chebyshev Series via FFTs

Chebyshev-Fourier transformation

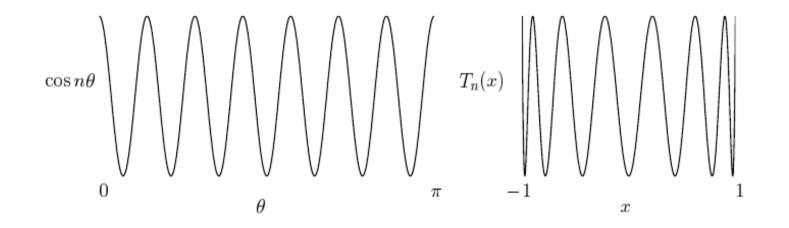


Fig. 8.2. The Chebyshev polynomial T_n can be interpreted as a sine wave "wrapped around a cylinder and viewed from the side".

Chebyshev via FFT

- This means that we can do **FFTs in equispaced points on** $\theta \in [0, 2\pi]$ instead of Chebyshev on non-equispaced nodes.
- Note that we want to extend this to θ ∈ [0, 2π] to be periodic and not θ ∈ [0, π], so we double the number of points and do the FFTs on vectors of length 2N.
- If f(x) can be extended analytically just outside of [-1, 1], then we get spectral accuracy.
- Intuition: Chebyshev polynomials are sine waves "wrapped around a cylinder and viewed from the side".
- One can approximate derivatives using the FFT; all that is needed is change of variables from x to θ using the chain rule.
- The chain of variables adds factors of the form (1 x²)^{-p/2} (where p is an integer) when converting from Fourier coefficients derivatives of g to derivatives of f.

Conclusions

Conclusions

Function Norms

- Consider a one-dimensional interval I = [a, b]. Standard norms for functions similar to the usual vector norms:
 - Maximum norm: $\|f(x)\|_{\infty} = \max_{x \in I} |f(x)|$
 - L_1 norm: $||f(x)||_1 = \int_a^b |f(x)| dx$
 - Euclidian L_2 norm: $||f(x)||_2 = \left[\int_a^b |f(x)|^2 dx\right]^{1/2}$
- Different function norms are not equivalent!
- An inner or scalar product (equivalent of dot product for vectors):

$$(f,g) = \int_a^b f(x)g^*(x)dx$$

Formally, function spaces are infinite-dimensional linear spaces.
 Numerically we always truncate and use a finite basis.

Conclusions

Discrete Function Norms

- Consider a set of *m* nodes x_i = a + ih with a constant grid spacing h = (b a)/m, and evaluate the function at those nodes pointwise
 f = {f(x₀), f(x₁), ..., f(x_m)}.
- We define the discrete "function norms" and "dot products", with periodic BCs:

$$\|f(x)\|_{2} \approx \left[h\sum_{i=0}^{m-1} |f(x_{i})|^{2}\right]^{1/2} = \sqrt{h} \|\mathbf{f}\|_{2},$$

$$\|f(x)\|_{1} \approx h\sum_{i=0}^{m-1} |f(x_{i})| = h \|\mathbf{f}\|_{1},$$

$$\|f(x)\|_{\infty} \approx \max_{i} |f(x_{i})| = \|\mathbf{f}\|_{\infty}$$

$$(f,g) \approx \mathbf{f} \cdot \mathbf{g} = h\sum_{i=0}^{m-1} f(x_{i})g^{*}(x_{i}).$$

Conclusions/Summary

- **Convolution** in real space becomes **multiplication** in Fourier space, and vice versa.
- Spectrally-accurate derivatives f^(ν) of analytic functions f can be done by multiplication by (ik)^ν in Fourier space, zeroing out the unmatched mode for even N and odd ν.
- Not all forms of operators and PDEs equal on paper are equal numerically. Choose the form that preserves the important properties of the continuum PDE: conservation laws, self-Hermitian operators, completeness (this is where understanding PDEs is crucial beyond superficial: functional analysis).
- Nonlinear PDEs can be discretized spectrally in space to a system of coupled nonlinear ODEs. Non-periodic domains can be handled by using orthogonal polynomials but boundary conditions need to be thought about some more!