An Introduction to Spectral Methods in Python

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The Method of Lines

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• Suppose we want to solve the linear advection equation:

$$\frac{\partial u}{\partial t} = c \frac{\partial u}{\partial x}$$

• Discretize space only

$$\frac{\partial}{\partial t}u_i(t) = c\frac{u_i(t) - u_{i-1}(t)}{\Delta x}$$

• This is a *coupled system* of ODEs:

$$\frac{\partial}{\partial t}\mathbf{u} = D\mathbf{u}$$
, for some matrix D

• Solve using ODE methods discussed earlier such as RK2

What do we Discretize?

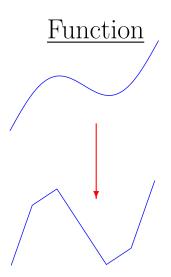
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What do we Discretize?

Equation

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$



Discretizing the Solution: The Function-Space Picture

• Represent solution as infinite-dimensional vector in Sobolev space

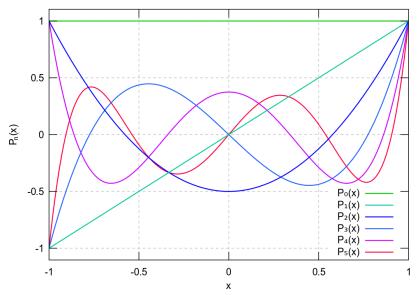
$$u(x) = \sum_{i=0}^{\infty} u_i \phi_i(x)$$

• To approximate, restrict to finite-dimensional subspace:

$$u(x) \approx \tilde{u}(x) = \sum_{i=0}^{N} u_i \phi_i(x)$$
 where $N \in \mathbb{N}$

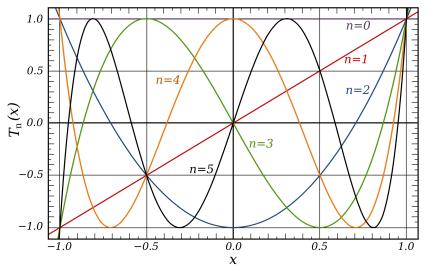
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A Legendre Basis



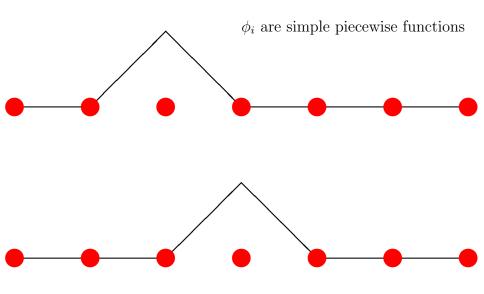
Source: Wikipedia

A Chebyshev Basis



Source: Wikipedia

Finite Differences in the Function Space Picture



Approximating the Equation

• E.g., for

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0,$$

In Finite Differences, demand:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_i^n - u_{i-1}^n}{\Delta x} = 0 \ \forall \ i, n \in \mathbb{Z}$$

In Galerkin Methods, Demand:

$$\int_{a}^{b} \left(\frac{\partial \tilde{u}}{\partial t} + c \frac{\partial \tilde{u}}{\partial x} \right) \phi_{i} w dx = 0 \ \forall \ i \in \mathbb{N}$$

Residual

Error

$$\epsilon = \|u - \tilde{u}\|$$
 generically, $\epsilon > 0$

$$\mathcal{R}_{i}^{n} = \frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} + c \frac{u_{i}^{n} - u_{i-1}^{n}}{\Delta x}$$
 or
$$\mathcal{R}_{i}^{n} = \left[\int_{a}^{b} \left(\frac{\partial \tilde{u}}{\partial t} + c \frac{\partial \tilde{u}}{\partial x} \right) \phi_{i} dx \right]_{t=t^{n}}$$
 often demand that

 $\mathcal{R}_i^n = 0$ identically $\forall i, n \in \mathbb{N}$

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Exercise

• Solve the equation

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0$$
 with $u(0, x) = \sin\left(e^{-(x-\pi)^2}\right)$ for $x \in [0, 2\pi]$

with periodic boundary conditions.

• Use a Fourier ansatz:

$$u(t,x) = \sum_{k=0}^{N} [a_k(t)\cos(kx) + b_k(t)\sin(kx)]$$
 for some $N \in \mathbb{N}$

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In no particular order:

- Numerical Recipes, by Press, Teukolsky, Vetterling, and Flannery
- Scientific Computing: An Introductory Survey, by Heath
- Introduction to Spectral Methods, by Grandclement (arXiv:gr-qc/0609020).
- Spectral Methods: Algorithms, Analysis, and Applications, by Shen, Tang, and Wang
- Spectral Methods in MATLAB, by Trefethen