

An Introduction to Spectral Methods in Python

Jonah M. Miller

Perimeter Institute

Tuesday, November 4, 2014

- 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:

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


- Solve using ODE methods discussed earlier such as RK2

What do we Discretize?

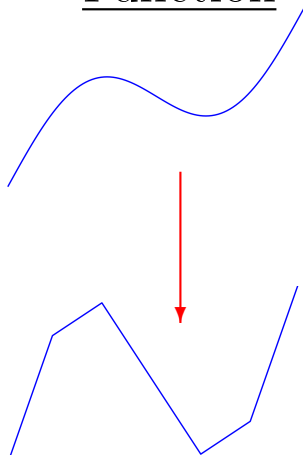
What do we Discretize?

Equation

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


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

Function



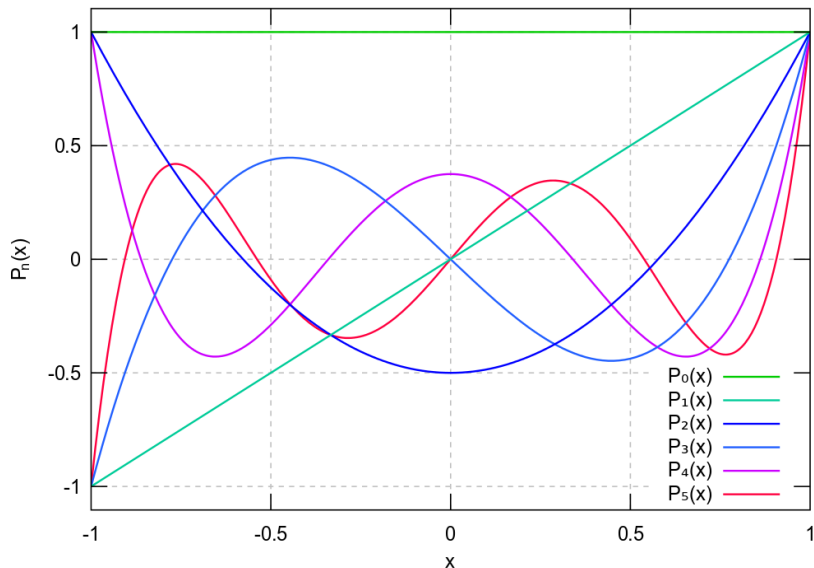
- Represent solution as infinite-dimensional vector in Sobolev space

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

- To approximate, restrict to finite-dimensional subspace:

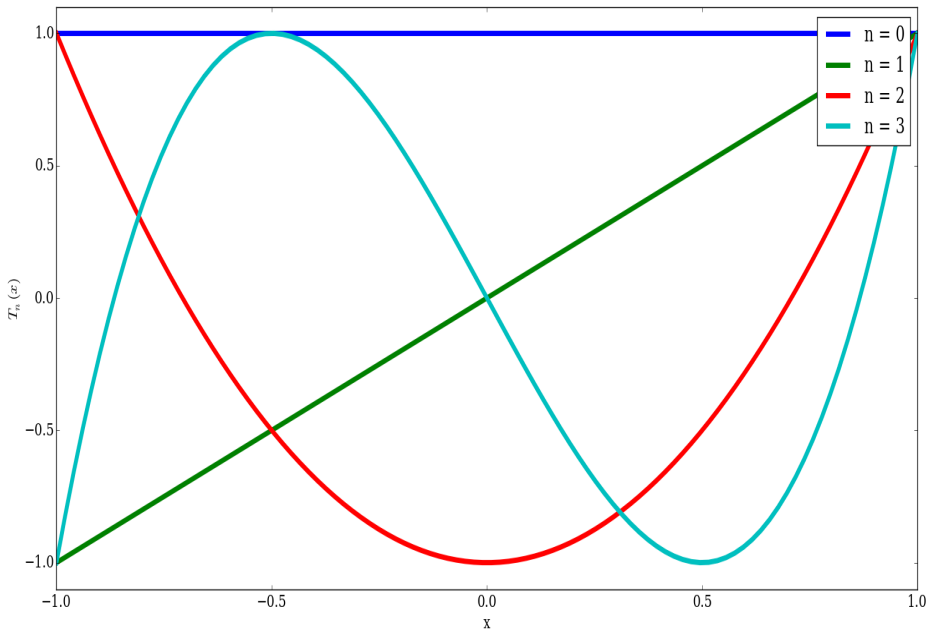
$$u(x) \approx \tilde{u}(x) = \sum_{i=0}^N u_i \phi_i(x) \text{ where } N \in \mathbb{N}$$

A Legendre Basis



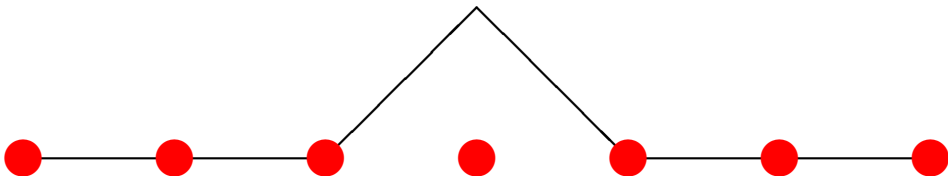
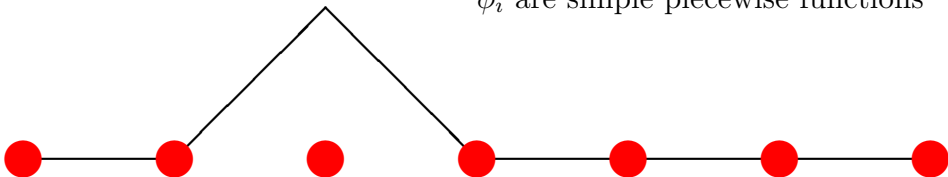
Source: Wikipedia

A Chebyshev Basis



Finite Differences in the Function Space Picture

ϕ_i are simple piecewise functions



Approximating the Equation

- E.g., for

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

In Finite Differences, demand:

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

In Galerkin Methods, Demand:

$$\int_a^b \left(\frac{\partial \tilde{u}}{\partial t} + c \frac{\partial \tilde{u}}{\partial x} \right) \phi_i w \, dx = 0 \quad \forall i \in \mathbb{N}$$

Error

$$\epsilon(t, x) = u(t, x) - \tilde{u}(t, x),$$

where $L[u] = 0$

generically, $\epsilon(x) > 0$

Residual

$$R(t, x) = \tilde{L}[\tilde{u}]$$

often demand that

$\mathcal{R}(t, x) = 0$ identically

Error

$$\epsilon_i^n = u(t, x) \Big|_{x=x^i}^{t=t^n} - u_i^{n+1},$$

or

$$\epsilon_i^n = \left[\int_a^b (u(t, x) - \tilde{u}(t, x)) \phi_i dx \right]_{t=t^n}$$

generically, $\epsilon_i^n > 0$

Residual

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

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

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

Example: The Galerkin Scheme

Suppose we want to solve

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} F[u] = 0$$

where F is an arbitrary (*nonlinear*) functional of u using the ansatz:

$$u(t, x) \approx \tilde{u} = \sum_{i=1}^N u_i(t) \phi_i(x) \quad N \in \mathbb{N}$$

and

$$F[u] \approx \tilde{F} = \sum_{i=1}^N F_i[u] \phi_i(x)$$

- Solve the equation

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

with periodic boundary conditions.

- Use a Fourier ansatz:

$$u(t, x) = a_0 + \sum_{k=1}^N [a_k(t) \cos(kx) + b_k(t) \sin(kx)] \text{ for some } N \in \mathbb{N}$$

- Assume the following inner product:

$$\langle a, b \rangle = \frac{1}{\pi} \int_{-\pi}^{\pi} a(x)b(x)dx$$

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 in MATLAB*, by Trefethen