Applied Mathematics 205

Unit 3. Numerical Calculus

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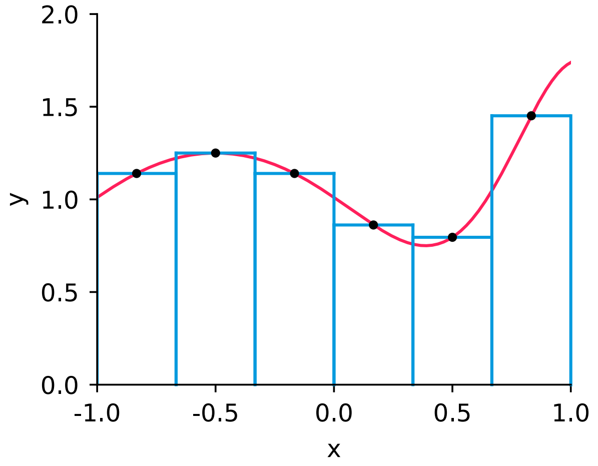
Motivation

- Since the time of Newton, calculus has been ubiquitous in science
- Calculus problems that arise in applications
  typically do not have closed-form solutions
- Numerical approximation is essential
- In this Unit we will consider
  - numerical integration
  - numerical differentiation
  - numerical methods for ordinary differential equations
  - numerical methods for partial differential equations

Integration

- The process of approximating a definite integral using a numerical method is called quadrature
- The Riemann sum suggests how to perform quadrature



- We will examine more accurate/efficient quadrature methods

Integration

- Question: Why is quadrature important?
- We know how to evaluate many integrals analytically,

$$\int_0^1 e^x \, \mathrm{d}x \qquad \text{or} \qquad \int_0^\pi \cos x \, \mathrm{d}x$$

- But how about

$$\int_1^{2000} \exp(\sin(\cos(\sinh(\cosh(\arctan(\log(x))))))) \, \mathrm{d}x$$

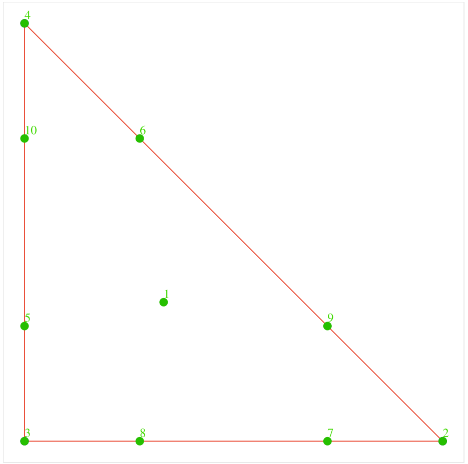
Integration

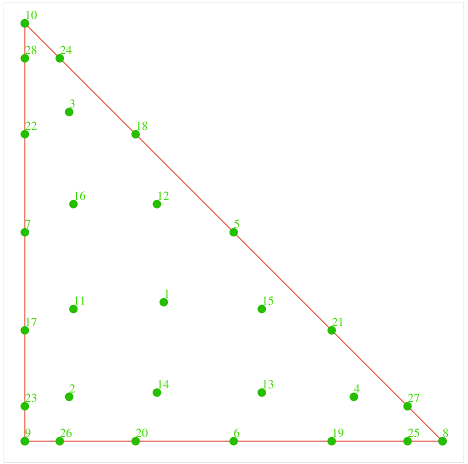
- We can numerically approximate this integral using `scipy.integrate.quad()`

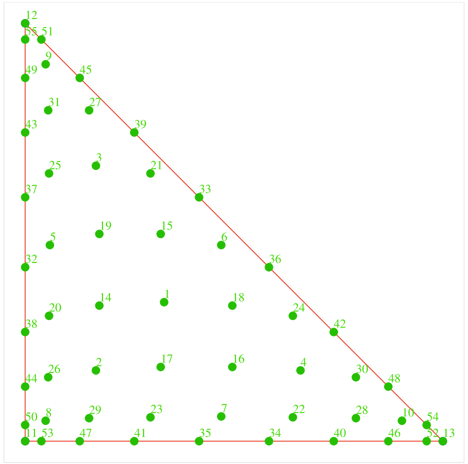
```
>>> import scipy
>>> from math import *
>>> def f(x):
...     return exp(sin(cos(sinh(cosh(atan(log(x)))))))
>>> scipy.integrate.quad(f, 1, 2000)
(1514.7806778270256, 4.231109731546272e-06)
```

Integration

- Quadrature also generalizes naturally to higher dimensions, and allows us to compute integrals on irregular domains
- For example, we can approximate an integral on a triangle based on a finite sum of samples at quadrature points



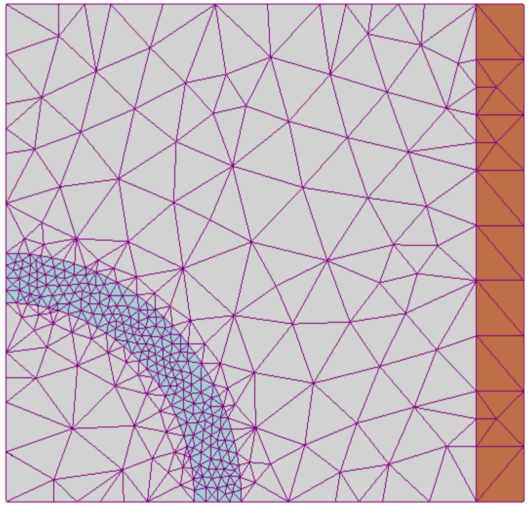




people.sc.fsu.edu/~jburkardt/cpp_src/triangle_fekete_rule_test

Integration

- And then evaluate integrals in complex geometries by triangulating the domain



Differentiation

- Numerical differentiation is another fundamental tool
- We have already discussed the most common, intuitive approach to numerical differentiation: finite differences
- Examples
  - $f'(x) = \frac{f(x+h)-f(x)}{h} + \mathcal{O}(h)$ forward difference
  - $f'(x) = \frac{f(x)-f(x-h)}{h} + \mathcal{O}(h)$ backward difference
  - $f'(x) = \frac{f(x+h)-f(x-h)}{2h} + \mathcal{O}(h^2)$ centered difference
  - $f''(x) = \frac{f(x+h)-2f(x)+f(x-h)}{h^2} + \mathcal{O}(h^2)$ centered, second derivative

Differentiation

- We will see how to derive these and other finite difference formulas and quantify their accuracy
- Wide range of choices, with trade-offs in terms of
  - accuracy
  - stability
  - complexity

Differentiation

- In Unit 0, we saw that finite differences can be sensitive to rounding error when h is "too small"
- But in most applications we obtain sufficient accuracy with h large enough that rounding error is still negligible
- Hence finite differences generally work very well and provide a very popular approach to solving problems involving derivatives

ODEs

- The most common situation in which we need to approximate derivatives is to solve differential equations
- Ordinary Differential Equations (ODEs):
  Differential equations involving functions of one variable
- Examples of problems
  - initial value problem (IVP) for a first order ODE
    $y'(t) = y^2(t) + t^4 - 6t$
    $y(0) = y_0$
  - boundary value problem (BVP) for a second order ODE
    $y''(x) + 2xy(x) = 1$
    $y(0) = y(1) = 0$

ODEs: IVP

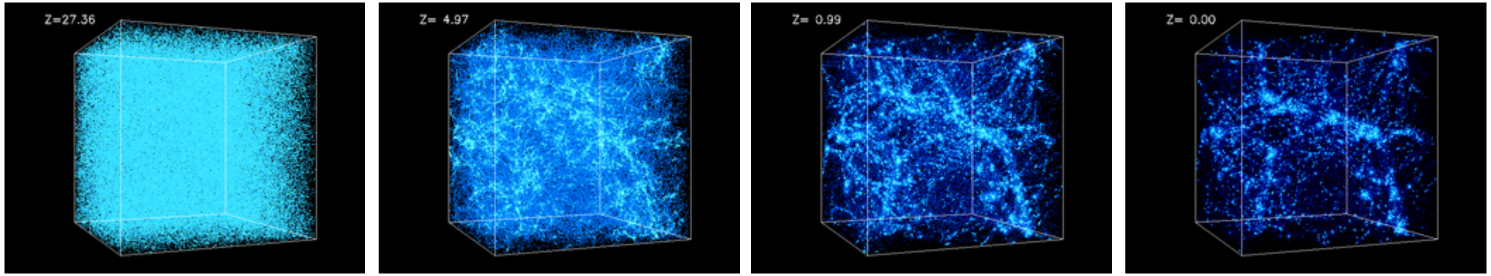
- Newton's second law of motion

$$y''(t) = \frac{F(t, y, y')}{m}, \quad y(0) = y_0, \quad y'(0) = v_0$$

  where $y(t) \in \mathbb{R}$ is the position of a particle of mass m at time $t \geq 0$
- This is a scalar ODE to simulate one particle
- An N-body problem involves a system of N interacting particles
- For example, F can be gravitational force due to other particles, and the force on particle i depends on positions of the other particles

ODEs: IVP

- N-body problems are the basis of many cosmological simulations
- Recall the galaxy formation simulations from Unit 0



- Computationally expensive when N is large!

ODEs: BVP

- Boundary value problems for ODEs are also important in many circumstances
- The steady-state heat equation for the temperature $u(x)$

$$-u''(x) = f(x), \quad u(-1) = 0, \quad u'(1) = 0$$

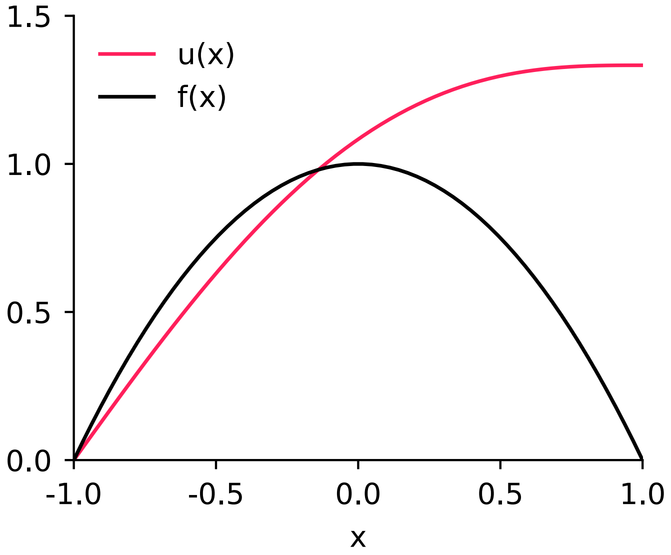
  - apply a heat source $f(x) = 1 - x^2$
  - impose zero temperature at $x = -1$
  - insulate at $x = 1$
- Here $u(x)$ is the temperature of a 1D rod

ODEs: BVP

- We can approximate the equation $-u''(x) = f(x)$ with finite differences

$$-\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} = f(x)$$

and impose $u(-1) = 0$ and $u(1) - u(1-h) = 0$



PDEs

- It is also natural to introduce time-dependence
- Now $u(x,t)$ is a function of x and t
  so derivatives of u are partial derivatives
  and we obtain a partial differential equation (PDE)
- The time-dependent heat equation for $u(x,t)$

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f(x)$$

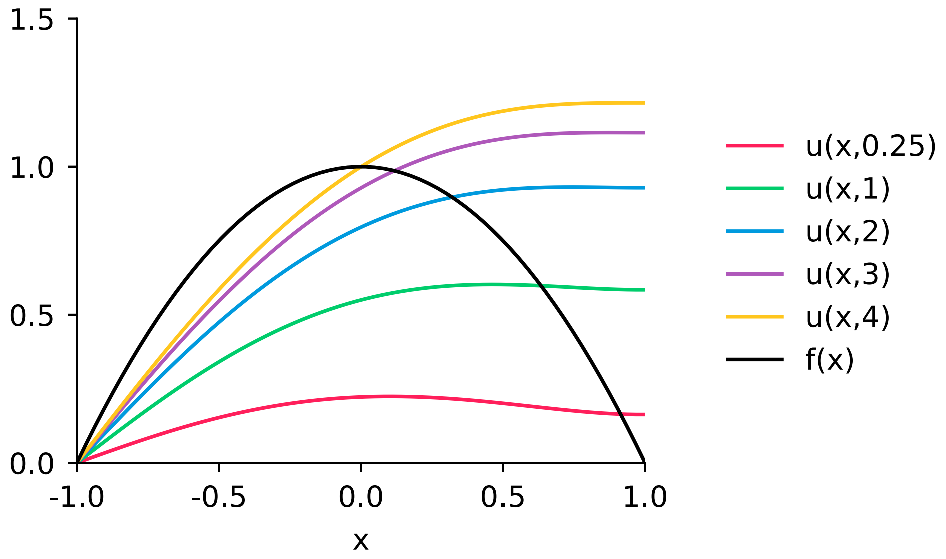
  with initial conditions $u(x,0) = 0$
  and boundary conditions $u(-1,t) = 0$, $\frac{\partial u}{\partial x}(1,t) = 0$
- This is an initial-boundary value problem (IBVP)

PDEs

- Again, we can approximate the equation $\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f(x)$ with finite differences

$$\frac{u(x,t)-u(x,t-\Delta t)}{\Delta t} - \frac{u(x+h,t)-2u(x,t)+u(x-h,t)}{h^2} = f(x)$$

and impose $u(x,0) = 0$, $u(-1,t) = 0$, and $u(1,t) - u(1-h,t) = 0$



PDEs

- This extends to 2D and 3D domains
- The time-dependent heat equation in a 3D domain $\Omega \subset \mathbb{R}^3$ for the temperature $u(x, y, z, t)$

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} - \frac{\partial^2 u}{\partial z^2} = f(x, y, z)$$

with initial conditions $u(x, y, z, 0) = u_0(x, y, z)$
and boundary conditions $u = 0$ on $\partial\Omega$

PDEs

- This equation is typically written as

$$\frac{\partial u}{\partial t} - \nabla^2 u = f(x, y, z)$$

  where $\nabla^2 u = \nabla \cdot \nabla u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$

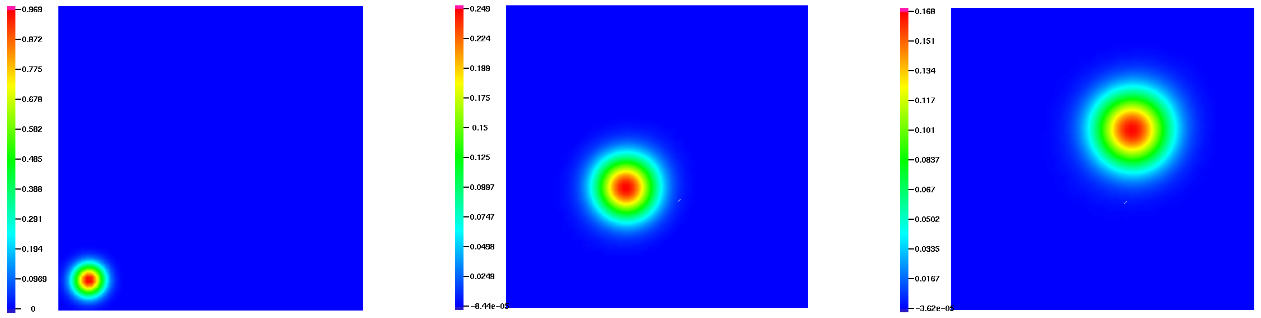
- Here we have
  - the Laplacian $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$
  - the gradient $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$

PDEs

- We can add a transport term to the heat equation to obtain the convection-diffusion equation

$$\frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u - \nabla^2 u = f(x, y)$$

- Now $u(x, t)$ models the concentration of some substance in a medium moving with velocity $\mathbf{w}(x, y, t) \in \mathbb{R}^2$



PDEs

- The Navier-Stokes equations describe the motion of viscous liquids

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u}$$

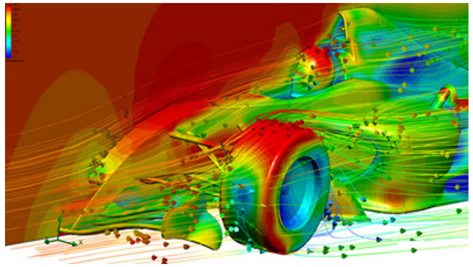
  together with the continuity equation (the liquid is incompressible)

$$\nabla \cdot \mathbf{u} = 0$$

  for the unknown velocity $\mathbf{u}$ and pressure p, where ν is the viscosity

PDEs

- Numerical methods for PDEs are a major topic in scientific computing
- Recall examples from Unit 0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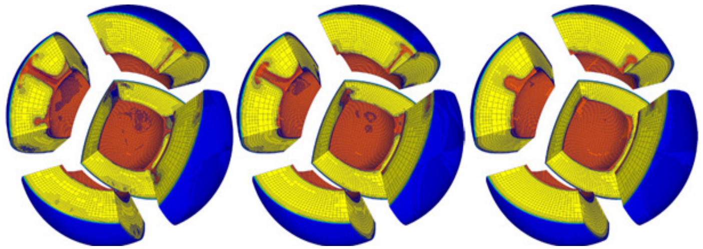

Geophysics

- In the course, we will focus on the finite difference method
- Alternative methods: finite element, finite volume, spectral, boundary element, particles, . . .

Summary

- Numerical calculus includes a wide range of topics and has important applications
- We will consider various algorithms and analyze their stability, accuracy, and efficiency

Quadrature

- Suppose we want to evaluate the integral $I(f) = \int_a^b f(x)\mathrm{d}x$
- We can proceed as follows
  - approximate f using a polynomial interpolant p_n
  - define $Q_n(f) = \int_a^b p_n(x)\mathrm{d}x$
    we can integrate polynomials exactly
- $Q_n(f)$ provides a quadrature formula,
  and we should have $Q_n(f) \approx I(f)$
- A quadrature rule based on an interpolant p_n
  at $n+1$ equally spaced points in $[a, b]$
  is known as Newton–Cotes formula of order n

Newton–Cotes Quadrature

- Let $x_k = a + kh, k = 0, 1, \dots, n$, where $h = (b-a)/n$
- We write the interpolant of f in the Lagrange form as

$$p_n(x) = \sum_{k=0}^{n} f(x_k) L_k(x), \quad \text{where} \quad L_k(x) = \prod_{i=0, i\neq k}^{n} \frac{x - x_i}{x_k - x_i}$$

- Then

$$Q_n(f) = \int_a^b p_n(x) \mathrm{d}x = \sum_{k=0}^{n} f(x_k) \int_a^b L_k(x) \mathrm{d}x = \sum_{k=0}^{n} w_k f(x_k)$$

where $w_k = \int_a^b L_k(x) \mathrm{d}x \in \mathbb{R}$ is the k-th quadrature weight

Newton–Cotes Quadrature

- Note that quadrature weights do not depend on f,
  so they can be precomputed and stored
  - trapezoid rule: $Q_1(f) = \frac{b-a}{2}\left[f(a) + f(b)\right]$
  - Simpson's rule: $Q_2(f) = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$
- We can develop higher-order Newton–Cotes formulas in the same way

Error Estimates

- Let $E_n(f) = I(f) - Q_n(f)$
- Then

$$\begin{aligned}
E_n(f) &= \int_a^b f(x)\mathrm{d}x - \sum_{k=0}^n w_k f(x_k) \\
&= \int_a^b f(x)\mathrm{d}x - \sum_{k=0}^n \left(\int_a^b L_k(x)\mathrm{d}x\right) f(x_k) \\
&= \int_a^b f(x)\mathrm{d}x - \int_a^b \left(\sum_{k=0}^n L_k(x) f(x_k)\right) \mathrm{d}x \\
&= \int_a^b f(x)\mathrm{d}x - \int_a^b p_n(x)\mathrm{d}x \\
&= \int_a^b (f(x) - p_n(x))\, \mathrm{d}x
\end{aligned}$$

- From Unit 1, we have an expression for $f(x) - p_n(x)$

Error Estimates

- Recall

$$f(x) - p_n(x) = \frac{f^{n+1}(\theta)}{(n+1)!}(x - x_0)\ldots(x - x_n)$$

- Hence

$$|E_n(f)| \leq \frac{M_{n+1}}{(n+1)!}\int_a^b |(x - x_0)(x - x_1)\cdots(x - x_n)|\mathrm{d}x$$

where $M_{n+1} = \max_{\theta\in[a,b]} |f^{n+1}(\theta)|$

Error Estimates

- For the trapezoid rule, the error bound is

$$|E_1(f)| \leq \frac{(b-a)^3}{12} M_2$$

- The bound for E_n depends directly on the integrand f (via M_{n+1})
- Just like with the Lebesgue constant, it is informative to be able to compare quadrature rules independently of the integrand

Error Estimates: Another Perspective

- Theorem: If Q_n integrates polynomials of degree n exactly, then $\exists C_n > 0$ such that $|E_n(f)| \leq C_n \min_{p \in \mathbb{P}_n} \|f - p\|_\infty$
- Proof: For any $p \in \mathbb{P}_n$, we have

$$\begin{aligned}
|E_n(f)| &= |I(f) - Q_n(f)| \\
&\leq |I(f) - I(p)| + |I(p) - Q_n(f)| \\
&= |I(f-p)| + |Q_n(f-p)| \\
&\leq \textstyle\int_a^b \mathrm{d}x \|f-p\|_\infty + \left(\sum_{k=0}^n |w_k|\right) \|f-p\|_\infty \\
&= C_n \|f-p\|_\infty
\end{aligned}$$

where $C_n = b - a + \sum_{k=0}^n |w_k|$ does not depend on p

Error Estimates

- Hence a convenient way to compare accuracy of quadrature rules is to compare the polynomial degree they integrate exactly
- Newton–Cotes of order n is based on polynomial interpolation, hence in general integrates polynomials of degree n exactly
- Also follows from the fact that $M_{n+1} = 0$ for a polynomial of degree n

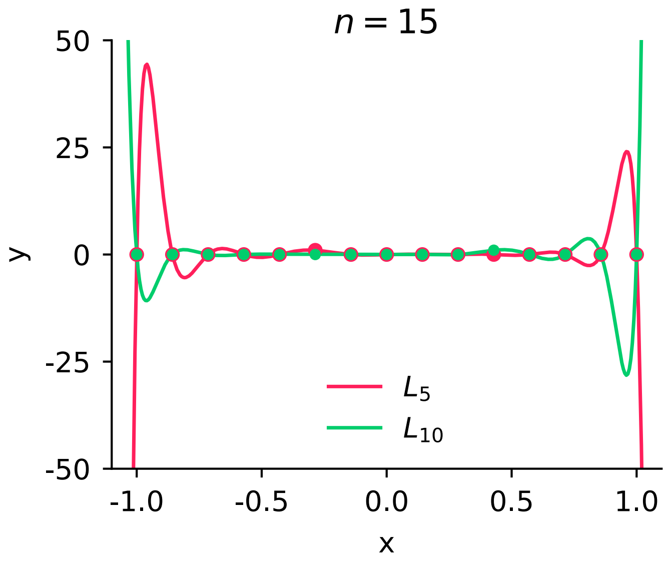
Runge's Phenomenon Again

- However, Newton–Cotes formulas are based on interpolation at equally spaced points
- Hence they're susceptible to Runge's phenomenon, and we expect them to be inaccurate for large n
- Question: How does this show up in our error bound?

$$|E_n(f)| \leq C_n \min_{p \in \mathbb{P}_n} \|f - p\|_\infty$$

Runge Phenomenon Again

- Answer: In the constant C_n
- Recall that $C_n = b - a + \sum_{k=0}^{n} |w_k|$, and that $w_k = \int_a^b L_k(x)\mathrm{d}x$



- If the L_k blow up due to equally spaced points, so does C_n

Runge Phenomenon Again

- In fact, we know that $\sum_{k=0}^{n} w_k = b - a$, why?
- This tells us that if all the w_k are positive, then

$$C_n = b - a + \sum_{k=0}^{n} |w_k| = b - a + \sum_{k=0}^{n} w_k = 2(b-a)$$

- If weights are positive, then C_n is a constant (independent of n) and the quadrature converges to the exact integral

$$Q_n(f) \to I(f) \quad \text{as } n \to \infty$$

Runge Phenomenon Again

- But with Newton–Cotes, quadrature weights become negative for $n > 8$ (in example above, $L_{10}(x)$ would clearly yield $w_{10} < 0$)
- Key point: Newton–Cotes is not useful for large n
- However, there are two natural ways to get quadrature rules that converge as $n \to \infty$
  - integrate piecewise polynomial interpolant
  - do not use equally spaced interpolation points
- We consider piecewise polynomial-based quadrature rules first

Composite Quadrature Rules

- Integrating a piecewise polynomial interpolant leads to a composite quadrature rule
- Suppose we divide $[a, b]$ into m subintervals, each of width $h = (b-a)/m$, and $x_i = a + ih$, $i = 0, 1, \ldots, m$
- Then we have

$$I(f) = \int_a^b f(x)\mathrm{d}x = \sum_{i=1}^{m} \int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x$$

Composite Trapezoid Rule

- Composite trapezoid rule: Apply trapezoid rule to each interval

$$\int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x \approx \frac{1}{2}h[f(x_{i-1}) + f(x_i)]$$

- The composite quadrature is denoted as

$$\begin{aligned} Q_{1,h}(f) &= \sum_{i=1}^{m} \frac{1}{2}h[f(x_{i-1}) + f(x_i)] \\ &= h\left[\frac{1}{2}f(x_0) + f(x_1) + \cdots + f(x_{m-1}) + \frac{1}{2}f(x_m)\right] \end{aligned}$$

Composite Trapezoid Rule

- Composite trapezoid rule error analysis

$$E_{1,h}(f) = I(f) - Q_{1,h}(f) = \textstyle\sum_{i=1}^{m} \left[\int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x - \frac{1}{2}h[f(x_{i-1}) + f(x_i)]\right]$$

- Hence,

$$\begin{aligned}
|E_{1,h}(f)| &\le \textstyle\sum_{i=1}^{m} \left|\int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x - \frac{1}{2}h[f(x_{i-1}) + f(x_i)]\right| \\
&\le \frac{h^3}{12} \sum_{i=1}^{m} \max_{\theta\in[x_{i-1},x_i]} |f''(\theta)| \\
&\le \frac{h^3}{12} m\|f''\|_\infty \\
&= \frac{h^2}{12}(b-a)\|f''\|_\infty
\end{aligned}$$

Composite Simpson Rule

- We can obtain composite Simpson's rule in the same way
- Suppose that $[a, b]$ is divided into $2m$ intervals by the points $x_i = a + ih,\ \ i = 0, \ldots, 2m$, where $h = (b - a)/2m$
- Applying Simpson's rule on each interval $[x_{2i-2}, x_{2i}]$, $i = 1, \ldots, m$ yields

$$\begin{aligned} Q_{2,h}(f) = \frac{h}{3}[&f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots \\ &+ 2f(x_{2m-2}) + 4f(x_{2m-1}) + f(x_{2m})] \end{aligned}$$

- See [examples/unit3/quadcomp.py] with composite trapezoid and Simpson's rules

Adaptive Quadrature

- Composite quadrature rules are very flexible, can be applied to intervals of variable sizes
- We should use smaller intervals where f varies rapidly, and larger intervals where f varies slowly
- This can be achieved by adaptive quadrature:
  1. Initialize to $m = 1$ (one interval)
  2. On each interval, evaluate quadrature rule and estimate quadrature error
  3. If error estimate is larger than a given tolerance on interval i, subdivide into two smaller intervals and return to step 2
- Question: How can we estimate the quadrature error on an interval?

Adaptive Quadrature

- One straightforward way to estimate quadrature error on interval i is to compare to a more refined result for interval i
- Let $I^i(f)$ denote the exact integral and $Q_h^i(f)$ denote quadrature approximation on interval i
- Let $\hat{Q}_h^i(f)$ denote a more refined quadrature approximation on interval i, e.g. obtained by subdividing interval i
- Then for the error on interval i, we have

$$|I^i(f) - Q_h^i(f)| \leq |I^i(f) - \hat{Q}_h^i(f)| + |\hat{Q}_h^i(f) - Q_h^i(f)|$$

- Suppose we can neglect $|I^i(f) - \hat{Q}_h^i(f)|$ so that we use $|\hat{Q}_h^i(f) - Q_h^i(f)|$ as a computable estimator for $|I^i(f) - Q_h^i(f)|$

Gauss Quadrature

- Next we consider the second approach to developing more accurate quadrature rules: unevenly spaced quadrature points
- Recall that we can compare accuracy of quadrature rules based on the polynomial degree that is integrated exactly
- So far, we have only used equally spaced points
- More accurate quadrature rules can be derived by choosing the x_i to maximize the degree of polynomials integrated exactly
- Resulting family of quadrature rules is called Gauss quadrature

Gauss Quadrature

- With $n + 1$ quadrature points and $n + 1$ quadrature weights, we have $2n + 2$ parameters to choose
- We might hope to integrate a polynomial with $2n + 2$ parameters, i.e. of degree $2n + 1$
- It can be shown that this is possible and leads to Gauss quadrature
- Again the idea is to integrate a polynomial interpolant, but we choose a specific set of interpolation points: Gauss quadrature points are roots of a Legendre polynomial

Gauss Quadrature

- Legendre polynomials $\{P_0, P_1, \ldots, P_n\}$ form an orthogonal basis for $\mathbb{P}_n$ in the L_2 inner product

$$\int_{-1}^{1} P_m(x)P_n(x)\mathrm{d}x = \begin{cases} \frac{2}{2n+1}, & m = n \\ 0, & m \neq n \end{cases}$$

Gauss Quadrature

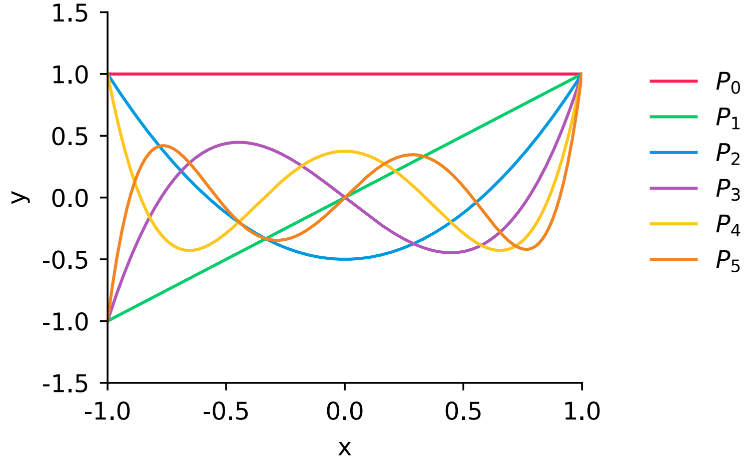
- Legendre polynomials satisfy a recurrence relation

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$$

- The first six Legendre polynomials



Gauss Quadrature

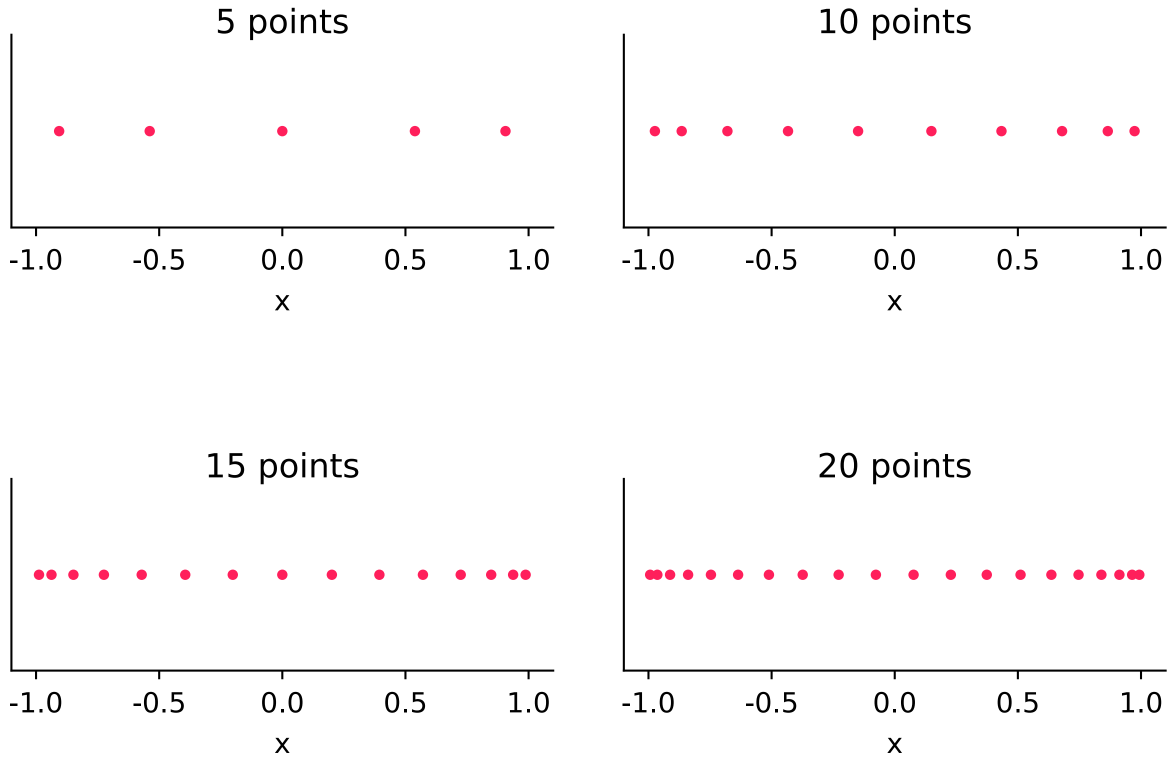
- We can find the roots of $P_n(x)$ and derive the n-point Gauss quadrature rule in the same way as for Newton–Cotes: integrate the Lagrange interpolant
- Gauss quadrature rules have been extensively tabulated for $x \in [-1, 1]$

Number of points	**Quadrature points**	**Quadrature weights**
1	0	2
2	$-1/\sqrt{3}, 1/\sqrt{3}$	$1, 1$
3	$-\sqrt{3/5}, 0, \sqrt{3/5}$	$5/9, 8/9, 5/9$
$\dots$	$\dots$	$\dots$

- Key point: Gauss quadrature weights are always positive, so Gauss quadrature converges as $n \to \infty$

Gauss Quadrature Points

- Points cluster toward ± 1 which prevents Runge's phenomenon!



Finite Differences

Finite Differences

- Finite differences approximate a derivative of function
$$f : \mathbb{R} \to \mathbb{R}$$
using samples of f on a finite set of points
- The points often form a uniform grid,
so the approximation at point x involves values
$$\ldots,\quad f(x-2h),\quad f(x-h),\quad f(x),\quad f(x+h),\quad f(x+2h),\quad \ldots$$

Finite Differences

- An approximation of the first derivative at point x can be derived from Taylor expansion about x evaluated at $x + h$

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \cdots$$

- Solving for $f'(x)$ we get the forward difference formula

$$\begin{aligned} f'(x) &= \frac{f(x+h) - f(x)}{h} - \frac{f''(x)}{2}h + \cdots \\ &\approx \frac{f(x+h) - f(x)}{h} \end{aligned}$$

- Here we neglected an $\mathcal{O}(h)$ term

Finite Differences

- The same expansion evaluated at $x - h$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{6}h^3 + \cdots$$

yields the backward difference formula

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

- Again, we neglected an $\mathcal{O}(h)$ term

Finite Differences

- Subtracting Taylor expansions for $f(x+h)$ and $f(x-h)$ gives the centered difference formula

$$\begin{aligned} f'(x) &= \frac{f(x+h)-f(x-h)}{2h} - \frac{f'''(x)}{6}h^2 + \cdots \\ &\approx \frac{f(x+h)-f(x-h)}{2h} \end{aligned}$$

- This one has a higher order, we neglected an $\mathcal{O}(h^2)$ term

Finite Differences

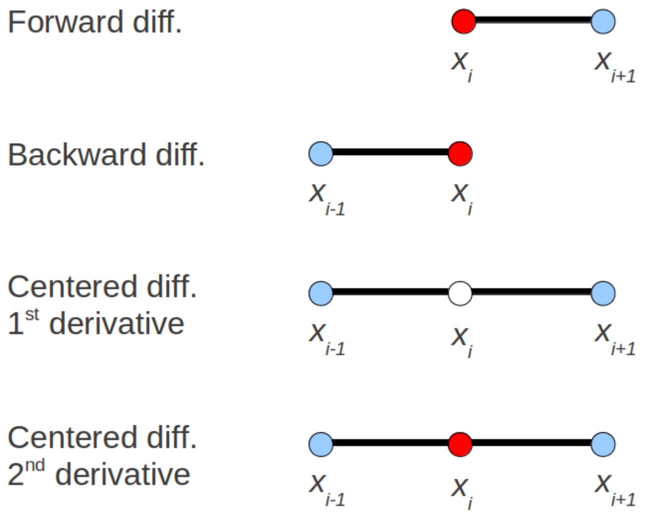
- Adding Taylor expansions for $f(x+h)$ and expansion for $f(x-h)$ gives the centered difference formula for the second derivative

$$\begin{aligned} f''(x) &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{f^{(4)}(x)}{12}h^2 + \cdots \\ &\approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \end{aligned}$$

- Again, we neglected an $\mathcal{O}(h^2)$ term

Finite Difference Stencils

- The pattern of points involved in a finite difference approximation is called a stencil
- Examples of stencils, x_i is the point of interest



Finite Differences

- By evaluating a Taylor expansion on stencils with more points, we can derive:
  - approximations with a higher order of accuracy
  - approximations for higher derivatives
- However, there is a more systematic way: differentiate an interpolant

Finite Differences

- Linear interpolant through $(x, f(x))$ and $(x+h, f(x+h))$ is

$$p_1(t) = f(x)\frac{x+h-t}{h} + f(x+h)\frac{t-x}{h}$$

- Differentiating p_1 gives

$$p_1'(t) = \frac{f(x+h) - f(x)}{h}$$

  which is the forward difference formula

- Exercise: Derive the backward difference formula using interpolation

Finite Differences

- Quadratic interpolant p_2 from interpolation points $x - h,\ x,\ x + h$ gives the centered difference formula for $f'(x)$:
  - differentiate p_2 to get a linear polynomial p_2'
  - evaluate $p_2'(x)$ to get centered difference formula for $f'(x)$
- Also, $p_2''(x)$ gives the centered difference formula for f''
- This approach can be applied to
  - higher degree interpolants (higher order, higher derivatives)
  - unevenly spaced points (adaptive approximations)

Differentiation Matrices

- So far we have talked about finite difference formulas to approximate $f'(x)$ at a single point x
- Now consider a grid $x_1, \ldots,\ x_n \in \mathbb{R}$ and vectors of
  - values $F = [f(x_1), \ldots,\ f(x_n)]^T \in \mathbb{R}^n$
  - derivatives $F' = [f'(x_1), \ldots,\ f'(x_n)]^T \in \mathbb{R}^n$
  - approximations $\tilde{F}' = [\tilde{f}'(x_1), \ldots,\ \tilde{f}'(x_n)]^T \in \mathbb{R}^n$
- Introduce a mapping

$$D : \mathbb{R}^n \to \mathbb{R}^n$$

  from values F to approximations $\tilde{F}'$

Differentiation Matrices

- Since the exact differentiation is a linear operation, it is natural to assume that D is a linear mapping, i.e. $D(\alpha F + \beta G) = \alpha DF + \beta DG$
- Then D corresponds to a square matrix $D \in \mathbb{R}^{n\times n}$ called a differentiation matrix
- Row i of D corresponds to the finite difference formula for $f'(x_i)$

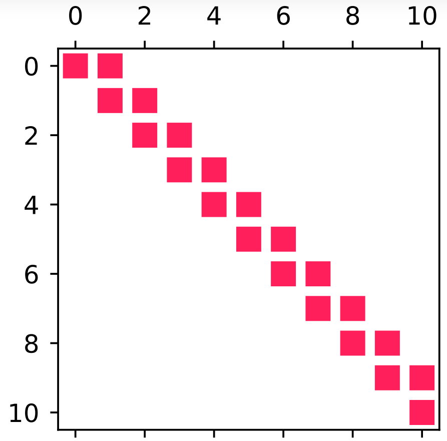
$$D_{(i,:)}F \approx f'(x_i)$$

- Note that discretizations of PDEs often involve nonlinear approximations of derivatives (will be considered later)

Example: Differentiation Matrix

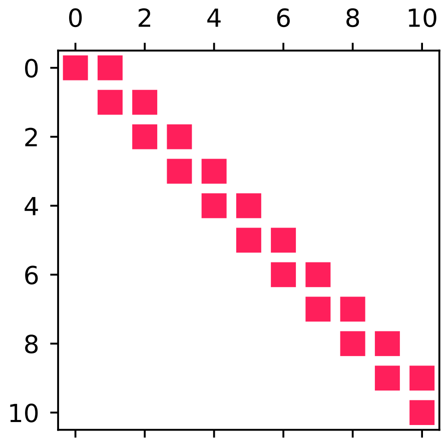
- Forward difference corresponds to a bidiagonal matrix with elements $D_{ii} = -\frac{1}{h}$, $D_{i,i+1} = \frac{1}{h}$

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> n = 11
>>> h = 1 / (n - 1)
>>> D = np.diag(-np.ones(n) / h) + np.diag(np.ones(n - 1) / h, 1
>>> plt.spy(D)
>>> plt.show()
```



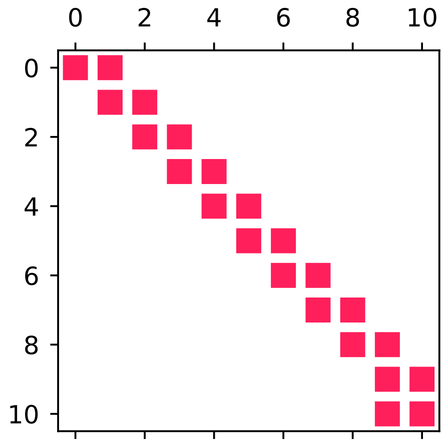
Example: Differentiation Matrix

- But the last row is incorrect, $D_{n,n+1} = \frac{1}{h}$ is ignored!



Example: Differentiation Matrix

- Boundary points need different formulas
- For example, use the backward difference in the last row
  $D_{n,n-1} = -\frac{1}{h}, \; D_{nn} = \frac{1}{h}$



- See [examples/unit3/diff_matr.py]

Initial Value Problems for ODEs

Initial Value Problems for ODEs

- An initial value problem for an ODE has the form

$$y'(t) = f(t, y(t)), \quad y(0) = y_0$$

  where
  - $y(t) \in \mathbb{R}^n$ is an unknown vector function
  - $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ is the right-hand side
  - $y(0) = y_0 \in \mathbb{R}^n$ is the initial condition
- The order of an ODE is the highest-order derivative that appears
- Therefore, $y'(t) = f(t, y)$ is a first order ODE

Initial Value Problems for ODEs

- We only consider first order ODEs since higher order problems can be transformed to first order by introducing extra variables
- For example, recall Newton's second law:

$$y''(t) = \frac{F(t, y, y')}{m}, \qquad y(0) = y_0, \quad y'(0) = v_0$$

- Introduce $v = y'$, then the original problem is equivalent to

$$\begin{aligned} v'(t) &= \frac{F(t, y, v)}{m} \\ y'(t) &= v(t) \end{aligned}$$

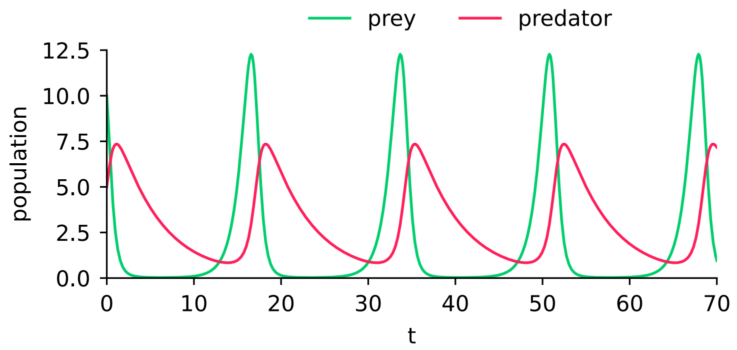
and $y(0) = y_0$, $v(0) = v_0$

Example: A Predator–Prey Model

- The Lotka–Volterra equation is a two-variable nonlinear ODE that models the evolution of populations of two species

$$y' = \begin{bmatrix} y_1(\alpha_1 - \beta_1 y_2) \\ y_2(-\alpha_2 + \beta_2 y_1) \end{bmatrix} \equiv f(y)$$

- Unknowns are the populations y_1 (prey) and y_2 (predator)
- Parameters are α_1 (birth rate), α_2 (death rate), β_1, and β_2 (interactions)
- See [examples/unit3/lotka_volterra.py]



ODEs in Python

- `scipy.integrate` has functions to solve initial value problems for ODEs
  - `odeint()`, uses `lsoda()` from FORTRAN library `odepack`
  - `solve_ivp()`, modern alternative with various methods

Forward Euler Method

- Suppose we want to compute an approximate solution to

$$y' = f(t, y), \quad y(0) = y_0$$

  at points $t_k = kh$ for $k = 0, 1, \ldots$
- Denote the approximation as $y_k \approx y(t_k)$
- Forward Euler method: use forward difference for y'

$$\frac{y_{k+1} - y_k}{h} = f(t_k, y_k), \quad k = 0, 1, \ldots$$

- See [examples/unit3/euler.py], Lotka-Volterra solved with forward Euler

Forward Euler Method

- Quadrature-based interpretation:
  integrating the ODE $y' = f(t,y)$ from t_k to t_{k+1} gives

$$y(t_{k+1}) = y(t_k) + \int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s$$

- Apply $n = 0$ Newton–Cotes quadrature to $\int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s$
  based on interpolation point t_k

$$\int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s \approx (t_{k+1} - t_k) f(t_k, y_k) = h f(t_k, y_k)$$

  to get the forward Euler method

$$y_{k+1} = y_k + h f(t_k, y_k)$$

Backward Euler Method

- We can derive other methods using the same quadrature-based approach
- Apply $n = 0$ Newton–Cotes quadrature to $\int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s$ based on interpolation point t_{k+1}

$$\int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s \approx (t_{k+1} - t_k) f(t_{k+1}, y_{k+1}) = hf(t_{k+1}, y_{k+1})$$

to get the backward Euler method

$$y_{k+1} = y_k + hf(t_{k+1}, y_{k+1})$$

Backward Euler Method

- Forward Euler method is an explicit method:
  we have an explicit formula for y_{k+1} in terms of y_k

$$y_{k+1} = y_k + hf(t_k, y_k)$$

- Backward Euler is an implicit method:
  we have to solve a nonlinear equation for y_{k+1}

$$y_{k+1} = y_k + hf(t_{k+1}, y_{k+1})$$

Backward Euler Method

- For example, approximate $y' = 2\sin(ty)$ using backward Euler
  - at the first step $k = 0$, we get
$$y_1 = y_0 + h\sin(t_1 y_1)$$
  - to compute y_1, let $F(y_1) = y_1 - y_0 - h\sin(t_1 y_1)$ and solve $F(y_1) = 0$ (e.g. using Newton's method)
- Implicit methods are more complicated and more computationally expensive to make one time step
- However, they can be more stable and accurate (to be seen shortly)

Trapezoid Method

- Higher-order quadrature leads to more accurate methods
- Apply $n = 1$ Newton–Cotes (trapezoid rule) to $\int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s$ based on interpolation points t_k, t_{k+1}

$$\int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s \approx \frac{h}{2}(f(t_k, y_k) + f(t_{k+1}, y_{k+1}))$$

to get the trapezoid method

$$y_{k+1} = y_k + \frac{h}{2}(f(t_k, y_k) + f(t_{k+1}, y_{k+1}))$$

One-Step Methods

- The three methods we have considered so far have the form

$$
\begin{aligned}
y_{k+1} &= y_k + h\Phi(t_k, y_k; h) && \text{(explicit)}\\
y_{k+1} &= y_k + h\Phi(t_{k+1}, y_{k+1}; h) && \text{(implicit)}\\
y_{k+1} &= y_k + h\Phi(t_k, y_k, t_{k+1}, y_{k+1}; h) && \text{(implicit)}
\end{aligned}
$$

  where the choice of the function Φ determines our method
- These are called one-step methods: y_{k+1} depends only on y_k
- In a multistep method, y_{k+1} depends on more values $y_k, y_{k-1}, y_{k-2}, \ldots$ (will be discussed briefly later)

Convergence

Convergence

- We now consider whether one-step methods converge to the exact solution as $h \to 0$
- Convergence is a crucial property since we want to be able to approach the exact solution at an arbitrary tolerance by taking a sufficiently small $h > 0$

Convergence

- Define the global error e_k
  as the total accumulated error at $t = t_k$

$$e_k = y(t_k) - y_k$$

- Define the truncation error T_k as the error introduced at one step k, starting from the exact solution, divided by h
- For example, the truncation error of an explicit one-step method is

$$T_k = \frac{y(t_{k+1}) - y(t_k)}{h} - \Phi(t_k, y(t_k); h)$$

Convergence

- The truncation error defined above determines
  the local error introduced by the ODE approximation
- For example, suppose $y_k = y(t_k)$, then for the case above we have

$$hT_k = y(t_{k+1}) - y_k - h\Phi(t_k, y_k; h) = y(t_{k+1}) - y_{k+1}$$

- Therefore, hT_k is the error introduced in one step of our ODE approximation
- The local error accumulates and determines the global error
- Now let's consider the global error of the Euler method in detail

Convergence

- Theorem: Suppose we apply forward Euler method to
$$y' = f(t, y)$$
for steps $k = 0, 1, \ldots, M-1$, where f satisfies a Lipschitz condition
$$|f(t,u) - f(t,v)| \leq L_f |u - v|,$$
where $L_f \in \mathbb{R}_{>0}$ is called a Lipschitz constant.
Then the global error is bounded as
$$|e_k| \leq \frac{\left(e^{L_f t_k} - 1\right)}{L_f} \left[\max_{0 \leq j \leq k-1} |T_j| \right], \quad k = 0, 1, \ldots, M$$
where T_j is the truncation error of the method

Convergence

Proof (1/3)

- From the definition of the truncation error, we have

$$y(t_{k+1}) = y(t_k) + hf(t_k, y(t_k); h) + hT_k$$

- Subtracting $y_{k+1} = y_k + hf(t_k, y_k; h)$ gives

$$e_{k+1} = e_k + h\left[f(t_k, y(t_k)) - f(t_k, y_k)\right] + hT_k$$

  therefore

  $|e_{k+1}| \leq |e_k| + hL_f|e_k| + h|T_k| = (1 + hL_f)|e_k| + h|T_k|$

Convergence

Proof (2/3)

- This gives a geometric progression, e.g. for $k = 2$ we have

$$\begin{aligned} |e_3| &\leq (1 + hL_f)|e_2| + h|T_2| \\ &\leq (1 + hL_f)((1 + hL_f)|e_1| + h|T_1|) + h|T_2| \\ &\leq (1 + hL_f)^2 h|T_0| + (1 + hL_f)h|T_1| + h|T_2| \\ &\leq h \left[\max_{0 \leq j \leq 2} |T_j| \right] \sum_{j=0}^{2} (1 + hL_f)^j \end{aligned}$$

- In general

$$|e_k| \leq h \left[\max_{0 \leq j \leq k-1} |T_j| \right] \sum_{j=0}^{k-1} (1 + hL_f)^j$$

Convergence

Proof (3/3)

- Use the formula for the sum

$$\sum_{j=0}^{k-1} r^j = \frac{1-r^k}{1-r}$$

with $r = (1 + hL_f)$, to get

$$|e_k| \leq \frac{1}{L_f}\left[\max_{0\leq j\leq k-1} |T_j|\right]\left((1+hL_f)^k - 1\right)$$

- Finally, use the bound $1 + hL_f \leq \exp(hL_f)$ to get the desired result $\square$

Convergence: Lipschitz Condition

- A simple case where we can calculate a Lipschitz constant is if $y \in \mathbb{R}$ and f is continuously differentiable
- Then from the mean value theorem we have

$$|f(t,u) - f(t,v)| = \left|\frac{\partial f}{\partial y}(t,\theta)\right| |u - v|,$$

for $\theta \in (u, v)$

- Therefore, a Lipschitz constant is given by

$$L_f = \max_{\substack{t \in [0,t_M] \\ \theta \in (u,v)}} |f_y(t,\theta)|$$

Convergence: Lipschitz Condition

- However, the Lipschitz condition is weaker, f does not have to be continuously differentiable
- For example, let $f(x) = |x|$, then $|f(x) - f(y)| = ||x| - |y|| \leq |x - y|$, and therefore $L_f = 1$

Convergence

- For a fixed t (i.e. $t = kh$, as $h \to 0$ and $k \to \infty$), the factor $(e^{L_f t} - 1)/L_f$ in the bound is a constant
- Hence the global convergence rate for each fixed t is given by the dependence of T_k on h
- Our proof was for forward Euler, but the same dependence of global error on local error holds in general
- We say that a method has order of accuracy p if

$$|T_k| = \mathcal{O}(h^p)$$

- From our error bound, ODE methods with order ≥ 1 are convergent

Order of Accuracy

- Forward Euler is first order accurate

$$
\begin{aligned}
T_k &= \frac{y(t_{k+1}) - y(t_k)}{h} - f(t_k, y(t_k)) \\
&= \frac{y(t_{k+1}) - y(t_k)}{h} - y'(t_k) \\
&= \frac{y(t_k) + hy'(t_k) + h^2 y''(\theta)/2 - y(t_k)}{h} - y'(t_k) \\
&= \frac{h}{2} y''(\theta)
\end{aligned}
$$

Order of Accuracy

- Backward Euler is first order accurate

$$\begin{aligned}
T_k &= \frac{y(t_{k+1}) - y(t_k)}{h} - f(t_{k+1}, y(t_{k+1})) \\
&= \frac{y(t_{k+1}) - y(t_k)}{h} - y'(t_{k+1}) \\
&= \frac{y(t_{k+1}) - y(t_{k+1}) + hy'(t_{k+1}) - h^2 y''(\theta)/2}{h} - y'(t_{k+1}) \\
&= -\frac{h}{2} y''(\theta)
\end{aligned}$$

Order of Accuracy

- Trapezoid method is second order accurate
- Let's prove this using a quadrature error bound, recall that

$$\frac{y(t_{k+1}) - y(t_k)}{h} = \frac{1}{h}\int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s$$

so the truncation error is

$$T_k = \frac{1}{h}\int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s - \frac{1}{2}\left[f(t_k, y(t_k)) + f(t_{k+1}, y(t_{k+1}))\right]$$

Order of Accuracy

- Then

$$\begin{aligned} T_k &= \frac{1}{h}\left[\int_{t_k}^{t_{k+1}} f(s, y(s))\mathrm{d}s - \frac{h}{2}\left(f(t_k, y(t_k)) + f(t_{k+1}, y(t_{k+1}))\right)\right] \\ &= \frac{1}{h}\left[\int_{t_k}^{t_{k+1}} y'(s)\mathrm{d}s - \frac{h}{2}\left(y'(t_k) + y'(t_{k+1})\right)\right] \end{aligned}$$

- Therefore, T_k is determined by the trapezoid quadrature rule error for the integrand y' on $t \in [t_k, t_{k+1}]$
- Recall that trapezoid quadrature rule error bound depends on $(b-a)^3 = (t_{k+1} - t_k)^3 = h^3$ and hence

$$T_k = \mathcal{O}(h^2)$$

Order of Accuracy

- The table below shows global error at $t = 1$ for $y' = y$, $y(0) = 1$ solved using forward Euler and trapezoid methods

h	E_{Euler}	E_{trap}
2.0e-2	2.67e-2	9.06e-05
1.0e-2	1.35e-2	2.26e-05
5.0e-3	6.76e-3	5.66e-06
2.5e-3	3.39e-3	1.41e-06

$$h \to h/2 \implies E_{\text{Euler}} \to E_{\text{Euler}}/2$$

$$h \to h/2 \implies E_{\text{trap}} \to E_{\text{trap}}/4$$

Stability

Stability

- So far we have discussed convergence of numerical methods for initial value problems for ODEs, i.e. asymptotic behavior as $h \to 0$
- It is also crucial to consider stability of numerical methods: for what values of h is the method stable?
- We want the method to be stable for as large a step size as possible
- Taking fewer larger steps can be more efficient

Stability

- In this context, the key idea is that we want our methods to inherit the stability properties of the ODE
- If an ODE is unstable, then we can't expect our discretization to be stable
- But if an ODE is stable, we want our discretization to be stable as well
- Hence we first discuss ODE stability, independent of numerical discretization

ODE Stability

- Consider an ODE $y' = f(t, y)$, and
  - let $y(t)$ be the solution for initial condition $y(0) = y_0$
  - let $\hat{y}(t)$ be the solution for initial condition $\hat{y}(0) = \hat{y}_0$
- The ODE is stable if:

  for every $\epsilon > 0$, $\exists \delta > 0$ such that

  $$\|\hat{y}_0 - y_0\| \le \delta \implies \|\hat{y}(t) - y(t)\| \le \epsilon$$

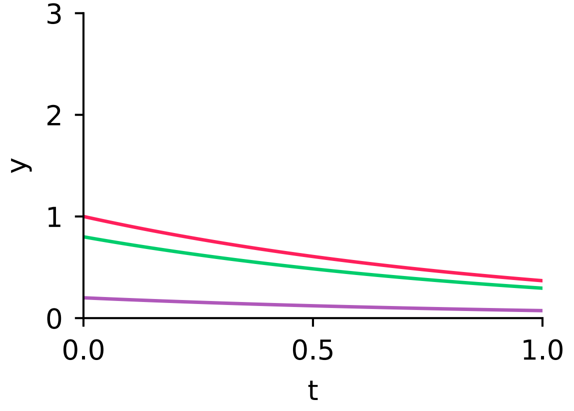
  for all $t \ge 0$
- Small input perturbation leads to small perturbation in the solution

ODE Stability

- A stronger form of stability, asymptotic stability: $\|\hat{y}(t) - y(t)\| \to 0$ as $t \to \infty$, perturbations decay over time
- These two definitions of stability are properties of the ODE, independent of any numerical algorithm
- In ODEs (and PDEs), it is standard to use stability to refer to sensitivity of both the mathematical problem and numerical approximations

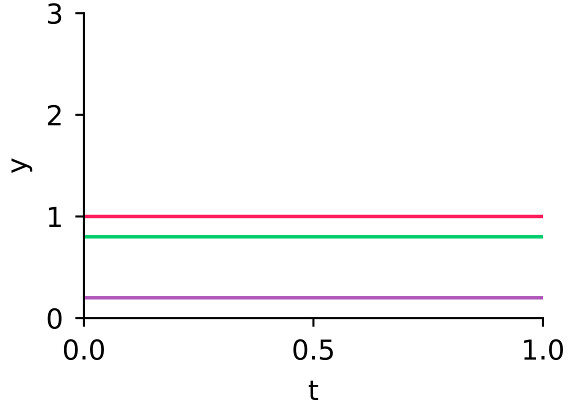
Example: ODE Stability

- Stability of $y' = \lambda y$ for different values of λ
  - solution $y = y_0 e^{\lambda t}$ for $y_0 = 1$
  - perturbed solution $\hat{y} = \hat{y}_0 e^{\lambda t}$ for $\hat{y}_0 = 0.9$
  - difference $|\hat{y} - y| = |\hat{y}_0 - y_0| e^{\lambda t}$



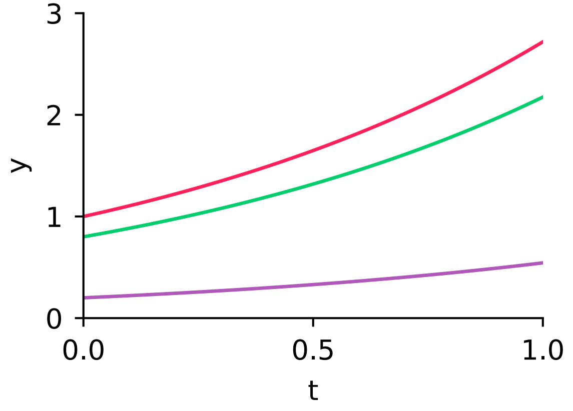
$\lambda = -1$

asymptotically stable



$\lambda = 0$

stable



$\lambda = 1$

unstable

ODE Stability

- More generally, we can allow λ to be a complex number: $\lambda = a + ib$
- Then $y(t) = y_0 e^{(a+ib)t} = y_0 e^{at} e^{ibt} = y_0 e^{at}(\cos(bt) + i \sin(bt))$
- The key issue for stability is now the sign of $a = \mathrm{Re}(\lambda)$
  - $\mathrm{Re}(\lambda) < 0 \implies$ asymptotically stable
  - $\mathrm{Re}(\lambda) = 0 \implies$ stable
  - $\mathrm{Re}(\lambda) > 0 \implies$ unstable

ODE Stability

- Understanding the stability of a scalar equation $y' = \lambda y$ can extend to the case $y' = Ay$, where $y \in \mathbb{R}^n$, $A \in \mathbb{R}^{n \times n}$
- Suppose that A is diagonalizable, so that we have the eigenvalue decomposition $A = V \Lambda V^{-1}$, where
  - $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, where the λ_j are eigenvalues
  - V is matrix with eigenvectors as columns, $v_1, v_2, \ldots, v_n$
- Then,

$$y' = Ay = V \Lambda V^{-1} y \implies V^{-1} y' = \Lambda V^{-1} y \implies z' = \Lambda z$$

where $z = V^{-1} y$ and $z_0 = V^{-1} y_0$

ODE Stability

- Hence we have n decoupled ODEs for z,
  and the stability of z_i is determined by λ_i for each i
- Since z and y are related by the matrix V,
  then if all z_i are stable then all y_i will also be stable
- If $\operatorname{Re}(\lambda_i) \leq 0$ for $i = 1, \ldots, n$ then $y' = Ay$ is a stable ODE
- Next we consider stability of numerical approximations to ODEs

ODE Stability

- Numerical approximation to an ODE is stable if:
  for every $\epsilon > 0$, $\exists \delta > 0$ such that
  $$\|\hat{y}_0 - y_0\| \leq \delta \implies \|\hat{y}_k - y_k\| \leq \epsilon$$
  for all $k \geq 0$
- Key idea: We want to develop numerical methods
  that mimic the stability properties of the exact solution
- That is, if the ODE is unstable,
  we should not expect the numerical approximation to be stable

Stability

- Since ODE stability is problem dependent, we need a standard test problem
- The standard test problem is the simple scalar ODE

$$y' = \lambda y$$

- Behavior of a discretization on this test problem gives insight into behavior in general
- Ideally, to reproduce stability of the ODE $y' = \lambda y$, we want our discretization to be stable for all $\mathrm{Re}(\lambda) \leq 0$

Stability: Forward Euler

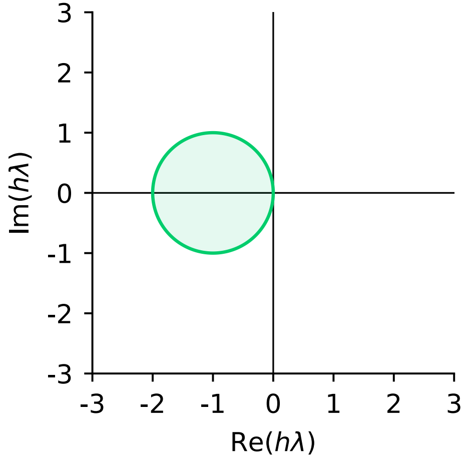
- Consider forward Euler discretization of $y' = \lambda y$

$$y_{k+1} = y_k + h\lambda y_k = (1 + h\lambda)y_k \implies y_k = (1 + h\lambda)^k y_0$$

- Here $1 + h\lambda$ is called the amplification factor
- Stability means $|1 + h\lambda| \leq 1$
- Let $h\lambda = a + ib$, then $|1 + a + ib|^2 \leq 1^2 \implies (1 + a)^2 + b^2 \leq 1$

Stability: Forward Euler

- Therefore, forward Euler is stable for $h\lambda \in \mathbb{C}$ inside the circle of radius 1 centered at $(-1, 0)$
- This is a subset of the left-half plane $\mathrm{Re}(h\lambda) \leq 0$



- We say that the forward Euler method is conditionally stable: if $\mathrm{Re}(\lambda) \leq 0$, we have to restrict h to ensure stability

Stability: Forward Euler

- For example, given $\lambda < 0$, we require

$$-2 \leq h\lambda \leq 0 \implies h \leq -2/\lambda$$

- Hence "larger negative λ" implies tighter restriction on h:

$$\begin{aligned} \lambda = -10 &\implies \quad h \leq 0.2 \\ \lambda = -200 &\implies \quad h \leq 0.01 \end{aligned}$$

- See [examples/unit3/euler_stab.py], forward Euler stability

Stability: Backward Euler

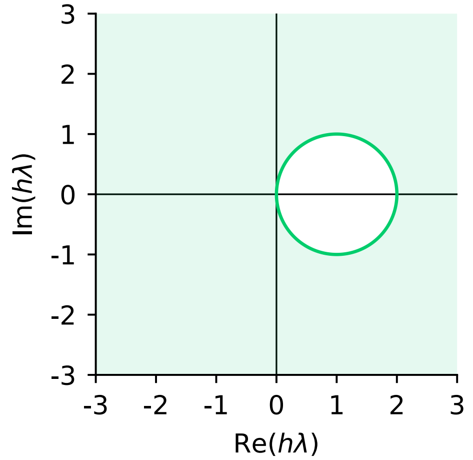
- In comparison, consider backward Euler for $y' = \lambda y$

$$y_{k+1} = y_k + h\lambda y_{k+1} \implies y_k = \left(\frac{1}{1-h\lambda}\right)^k y_0$$

- Here the amplification factor is $\frac{1}{1-h\lambda}$
  and the stability condition is $\frac{1}{|1-h\lambda|} \leq 1$

Stability: Backward Euler

- Let $h\lambda = a + ib$, then $1^2 \leq |1 - (a + ib)|^2$, i.e. $(1 - a)^2 + b^2 \geq 1$



- If $\mathrm{Re}(\lambda) \leq 0$, this is satisfied for any $h > 0$
- We say that the backward Euler method is unconditionally stable: if $\mathrm{Re}(\lambda) \leq 0$, no restriction on h for stability

Stability

- Generally, implicit methods have larger stability regions than explicit and therefore allow us to take larger time steps
- But explicit methods require less work per step since we do not need to solve for y_{k+1}
- Therefore there is a tradeoff: the choice of method should depend on the problem

Stability Regions

ODE

$y' = \lambda y$

$y(t) = y_0 e^{\lambda t}$

$|e^{\lambda}| \leq 1$

forward Euler

$y_{k+1} = y_k + h\lambda y_k$

$y_k = y_0(1 + h\lambda)^k$

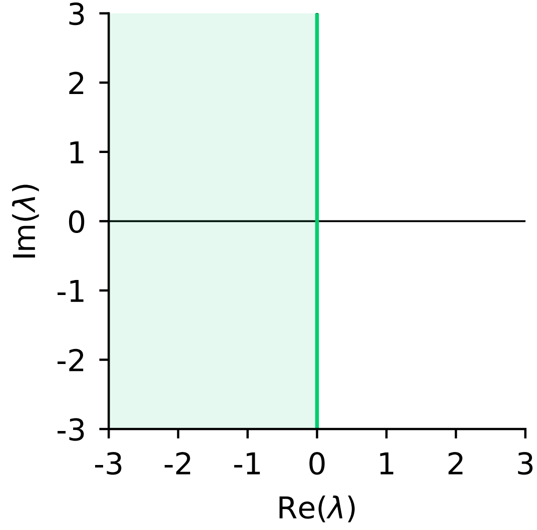
$|1 + h\lambda| \leq 1$

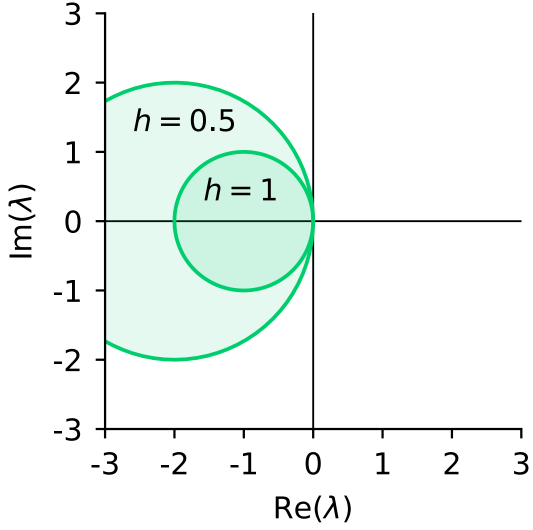
backward Euler

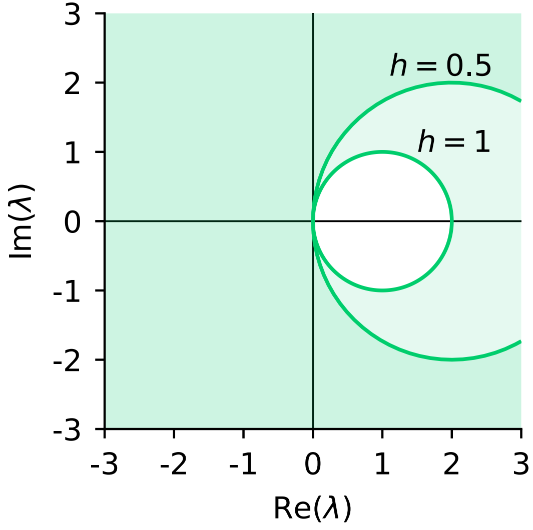
$y_{k+1} = y_k + h\lambda y_{k+1}$

$y_k = y_0/(1 - h\lambda)^k$

$|1/(1 - h\lambda)| \leq 1$







Runge–Kutta Methods

- Runge–Kutta (RK) methods are a popular class of one-step methods
- Aim to achieve higher order accuracy by combining evaluations of f at several points in $[t_k, t_{k+1}]$
- RK methods all fit within a general framework, which can be described in terms of Butcher tableaus
- We will first consider two RK examples: two evaluations of f and four evaluations of f
- Extra reading: Butcher, 1996. A history of Runge-Kutta methods

Runge–Kutta Methods

- A family of Runge–Kutta methods with two intermediate evaluations is defined by

$$\begin{aligned} k_1 &= f(t_k, y_k) \\ k_2 &= f(t_k + \alpha h, y_k + \beta h k_1) \\ y_{k+1} &= y_k + h(a k_1 + b k_2) \end{aligned}$$

- Forward Euler method is a member of this family, with $a = 1$ and $b = 0$
- It can be shown that certain combinations of a, b, α, β yield a second-order method

Runge–Kutta Methods

- Second-order methods with two stages
  - midpoint method ($\alpha = \beta = 1/2$, $a = 0$, $b = 1$)

$$y_{k+1} = y_k + hf\big(t_k + \tfrac{1}{2}h,\ y_k + \tfrac{1}{2}hf(t_k, y_k)\big)$$

  - Heun's method ($\alpha = \beta = 1$, $a = b = 1/2$)

$$y_{k+1} = y_k + \tfrac{1}{2}h[f(t_k, y_k) + f(t_k + h, y_k + hf(t_k, y_k))]$$

  - Ralston's method ($\alpha = 2/3$, $\beta = 2/3$, $a = 1/4$, $b = 3/4$)

$$y_{k+1} = y_k + \tfrac{1}{4}h[f(t_k, y_k) + 3f(t_k + \tfrac{2h}{3}, y_k + \tfrac{2h}{3}f(t_k, y_k))]$$

- See [examples/unit3/rk_order2.py]

Runge–Kutta Methods

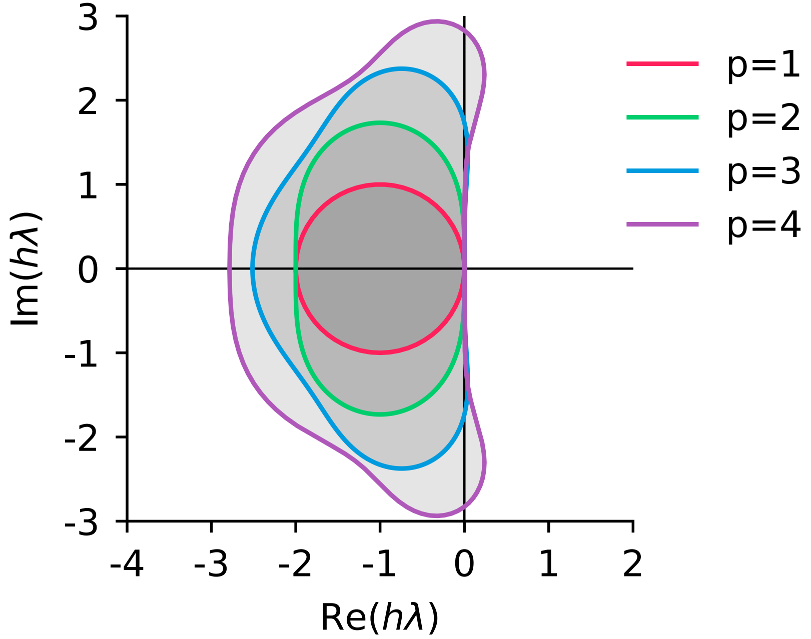
- The classical fourth-order Runge-Kutta method RK4 (available in `scipy.integrate.solve_ivp`)

$$
\begin{aligned}
k_1 &= f(t_k, y_k) \\
k_2 &= f(t_k + h/2, y_k + hk_1/2) \\
k_3 &= f(t_k + h/2, y_k + hk_2/2) \\
k_4 &= f(t_k + h, y_k + hk_3) \\
y_{k+1} &= y_k + \tfrac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}
$$

- It can be shown that the truncation error of RK4 is $T_k = \mathcal{O}(h^4)$

Runge–Kutta Methods: Stability

- Stability regions of p-stage Runge–Kutta methods of order p (do not depend on a particular method)



Butcher tableau

- Any explicit Runge–Kutta method with $s + 1$ stages can be represented using a triangular grid of coefficients called the Butcher tableau

$$\begin{array}{c|ccccc}
\alpha_0 & & & & & \\
\alpha_1 & \beta_{1,0} & & & & \\
\vdots & \vdots & & & & \\
\alpha_s & \beta_{s,0} & \beta_{s,1} & \dots & \beta_{s,s-1} & \\
\hline
 & \gamma_0 & \gamma_1 & \dots & \gamma_{s-1} & \gamma_s
\end{array}$$

- The i-th intermediate step is

$$k_i = f(t_k + \alpha_i h, y_k + h \textstyle\sum_{j=0}^{i-1} \beta_{i,j} k_j)$$

- The solution is updated as

$$y_{k+1} = y_k + h \textstyle\sum_{j=0}^{s} \gamma_j k_j$$

Richardson Extrapolation

- Richardson extrapolation is a general approach to analyze error and improve accuracy
- Treats the approximation as a “black box”
- Assume that $Y(h)$ is an approximation to y that depends on a discretization parameter $h > 0$ and the error has the form

$$Y(h) - y = Ch^p + \mathcal{O}(h^{p+1})$$

- Some parameters here may be known or unknown
  - exact solution y
  - order of accuracy p
  - factor of the leading error term C

Richardson Extrapolation

- We can evaluate $Y(h)$ for various h to eliminate the unknowns
- For example, if p is known we can evaluate $Y(2h)$ and $Y(h)$

$$Y(2h) - y = C2^p h^p + \mathcal{O}(h^{p+1})$$
$$Y(h) - y = Ch^p + \mathcal{O}(h^{p+1})$$

Richardson Extrapolation

- If we multiply the second equation by 2^p

$$Y(2h) - y = C2^p h^p + \mathcal{O}(h^{p+1})$$
$$2^p(Y(h) - y) = C2^p h^p + \mathcal{O}(h^{p+1})$$

and eliminate $C2^p h^p$, we get a higher-order approximation to y

$$y = \frac{1}{2^p - 1}\left[2^p Y(h) - Y(2h)\right] + \mathcal{O}(h^{p+1})$$

- The corresponding error estimate is

$$Y(h) - y = \frac{1}{2^p - 1}\left[Y(2h) - Y(h)\right] + \mathcal{O}(h^{p+1})$$

Error Estimation

- How can we compute the solution error without knowing the exact solution?
- Two approaches to estimate the error
  - Richardson extrapolation
  - include an error estimate in the derivation of the method

Error Estimation

- First approach: Richardson extrapolation
- Let $Y(h)$ be an approximation to $y(t)$ by a Runge–Kutta method of order p with a time step h

$$Y(h) - y(t) = Ch^p + \mathcal{O}(h^{p+1})$$

- Evaluate $Y(h)$ and $Y(h/2)$ to construct an approximation of order $p+1$

$$y(t) = \frac{1}{2^p - 1}[2^p Y(h/2) - Y(h)] + \mathcal{O}(h^{p+1})$$

- The corresponding error estimate is

$$Y(h/2) - y(t) = \frac{1}{2^p - 1}[Y(h) - Y(h/2)] + \mathcal{O}(h^{p+1})$$

- See [examples/unit3/richardson.py] and [examples/unit3/richardson2.py] applying Richardson extrapolation to each step of forward Euler (i.e. $t = h$)

Error Estimation

- Second approach: derive Butcher tableaus with an additional higher-order formula for estimating error
- Fehlberg's order 4(5) method RKF45
  - y_{k+1} is order 4, $\hat{y}_{k+1}$ is order 5, $y_{k+1} - \hat{y}_{k+1}$ is an error estimate

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{4} & \frac{1}{4} & & & & & \\
\frac{3}{8} & \frac{3}{32} & \frac{9}{32} & & & & \\
\frac{12}{13} & \frac{1932}{2197} & -\frac{7200}{2197} & \frac{7296}{2197} & & & \\
1 & \frac{439}{216} & -8 & \frac{3680}{513} & -\frac{845}{4104} & & \\
\frac{1}{2} & \frac{-8}{27} & 2 & \frac{-3544}{2565} & \frac{1859}{4104} & \frac{-11}{40} & \\
\hline
y_{k+1} & \frac{25}{216} & 0 & \frac{1408}{2565} & \frac{2197}{4104} & -\frac{1}{5} & 0 \\
\hat{y}_{k+1} & \frac{16}{135} & 0 & \frac{6656}{12825} & \frac{28561}{56430} & -\frac{9}{50} & \frac{2}{55}
\end{array}
$$

- Fehlberg, 1969. Low-order classical Runge-Kutta formulas with stepsize control and their application to some heat transfer problems. NASA

Higher-Order Methods

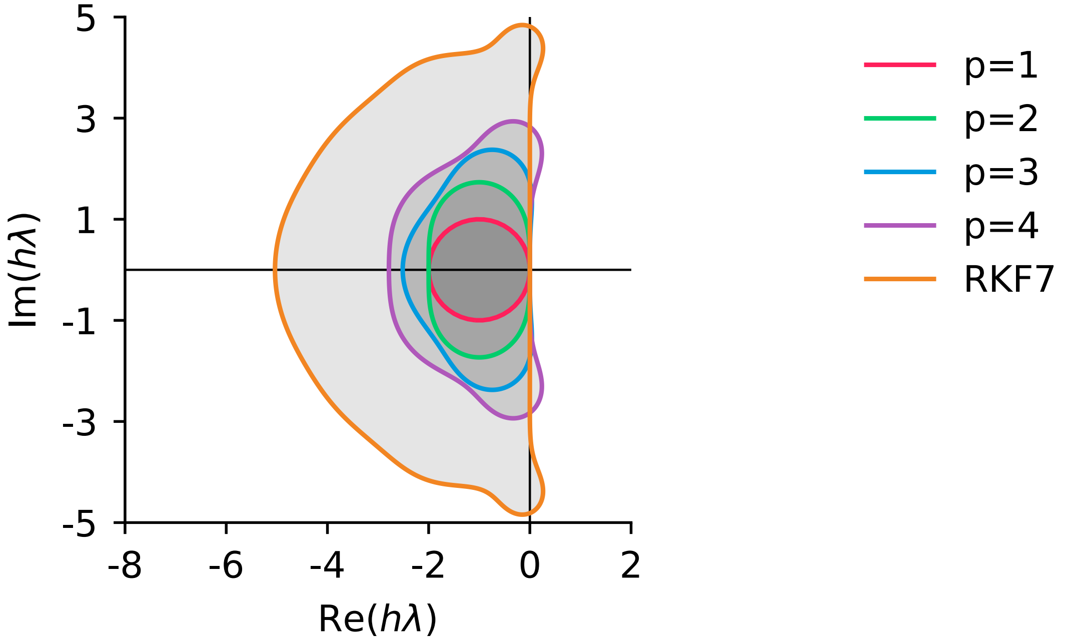
- Fehlberg's order 7(8) method RKF78

$$
\begin{array}{c|ccccccccccccc}
0 & & & & & & & & & & & & & \\
\frac{2}{27} & \frac{2}{27} & & & & & & & & & & & & \\
\frac{1}{9} & \frac{1}{36} & \frac{1}{12} & & & & & & & & & & & \\
\frac{1}{6} & \frac{1}{24} & 0 & \frac{1}{8} & & & & & & & & & & \\
\frac{5}{12} & \frac{5}{12} & 0 & -\frac{25}{16} & \frac{25}{16} & & & & & & & & & \\
\frac{1}{2} & \frac{1}{20} & 0 & 0 & \frac{1}{4} & \frac{1}{5} & & & & & & & & \\
\frac{5}{6} & -\frac{25}{108} & 0 & 0 & \frac{125}{108} & -\frac{65}{27} & \frac{125}{54} & & & & & & & \\
\frac{1}{6} & \frac{31}{300} & 0 & 0 & 0 & \frac{61}{225} & -\frac{2}{9} & \frac{13}{900} & & & & & & \\
\frac{2}{3} & 2 & 0 & 0 & -\frac{53}{6} & \frac{704}{45} & -\frac{107}{9} & \frac{67}{90} & 3 & & & & & \\
\frac{1}{3} & -\frac{91}{108} & 0 & 0 & \frac{23}{108} & -\frac{976}{135} & \frac{311}{54} & -\frac{19}{60} & \frac{17}{6} & -\frac{1}{12} & & & & \\
1 & \frac{2383}{4100} & 0 & 0 & -\frac{341}{164} & \frac{4496}{1025} & -\frac{301}{82} & \frac{2133}{4100} & \frac{45}{82} & \frac{45}{164} & \frac{18}{41} & & & \\
0 & \frac{3}{205} & 0 & 0 & 0 & 0 & -\frac{6}{41} & -\frac{3}{205} & -\frac{3}{41} & \frac{3}{41} & \frac{6}{41} & 0 & & \\
1 & -\frac{1777}{4100} & 0 & 0 & -\frac{341}{164} & \frac{4496}{1025} & -\frac{289}{82} & \frac{2193}{4100} & \frac{51}{82} & \frac{33}{164} & \frac{12}{41} & 0 & 1 & \\
\hline
y_{k+1} & \frac{41}{840} & 0 & 0 & 0 & 0 & \frac{34}{105} & \frac{9}{35} & \frac{9}{35} & \frac{9}{280} & \frac{9}{280} & \frac{41}{840} & 0 & 0 \\
\hat{y}_{k+1} & 0 & 0 & 0 & 0 & 0 & \frac{34}{105} & \frac{9}{35} & \frac{9}{35} & \frac{9}{280} & \frac{9}{280} & 0 & \frac{41}{840} & \frac{41}{840}
\end{array}
$$

- See implementation in [examples/unit3/fehlberg.py]
- Fehlberg, 1968. Classical fifth-, sixth-, seventh-, and eighth-order Runge-Kutta formulas with stepsize control. NASA

Higher-Order Methods: Stability

- Stability region of Fehlberg's order 7 method (13 stages) compared to order p Runge–Kutta methods



Stiff systems

- A system of linear ODEs

$$y' = Ay$$

  is called stiff if the eigenvalues of A differ greatly in magnitude
- Recall that if $A = V\Lambda V^{-1}$ with a diagonal matrix of eigenvalues Λ, then substitution $y = Vz$ reduces the system to $z' = \Lambda z$. Therefore, eigenvalues determine the timescales
- If the differences in eigenvalues are large, we need to resolve multiple timescales simultaneously

Stiff systems

- Suppose we are interested only in the slow components of the solution and can ignore the fast components
- However, an explicit method will need to resolve the fast components to avoid instability
- Therefore, it may be beneficial to use an implicit method for stiff systems

Stiff systems

- From a practical point of view, an ODE is considered stiff if there is a significant benefit in using an implicit method instead of explicit
- In particular, the time step required for stability is much smaller than what is required for accuracy
- Consider $y' = Ay$, $y_0 = [1, 0]^T$ where

$$A = \begin{bmatrix} 998 & 1998 \\ -999 & -1999 \end{bmatrix}$$

which has $\lambda_1 = -1$, $\lambda_2 = -1000$ and exact solution

$$y(t) = \begin{bmatrix} 2e^{-t} - e^{-1000t} \\ -e^{-t} + e^{-1000t} \end{bmatrix}$$

- See [examples/unit3/stiff.py] and [examples/unit3/stiff2.py]

Multistep Methods

- To obtain a high-order approximation one-step methods use multiple function evaluations
- Can we reuse data from earlier time steps instead?
- This is the idea of multistep methods

$$y_{k+1} = \sum_{i=1}^{m} \alpha_i y_{k+1-i} + h \sum_{i=0}^{m} \beta_i f(t_{k+1-i}, y_{k+1-i})$$

- If $\beta_0 = 0$ then the method is explicit
- Interpolate the solution and integrate the interpolant to derive the parameters

Multistep Methods

- See [examples/unit3/adams.py], second-order Adams–Bashforth method
- Question: Multistep methods require data from several earlier time steps, so how do we initialize?
- Answer: The standard approach is to use a one-step method and then move to multistep after collecting enough data
- Advantages of one-step methods over multistep
  - one-step methods are "self-starting", only need the initial condition
  - easier to adapt the time step size

Boundary Value Problems for ODEs

Boundary Value Problems for ODEs

- Consider a second-order linear ODE

$$-\alpha u''(x) + \beta u'(x) + \gamma u(x) = f(x)$$

  for $x \in [a, b]$ with given parameters $\alpha, \beta, \gamma \in \mathbb{R}$ and function $f : \mathbb{R} \to \mathbb{R}$

- The terms in this ODE have standard names
  - diffusion term $-\alpha u''(x)$
  - advection term $\beta u'(x)$
  - reaction term $\gamma u(x)$
  - source term $f(x)$

Boundary Value Problems for ODEs

- A boundary value problem (BVP) for a second-order linear ODE consists of

$$-\alpha u''(x) + \beta u'(x) + \gamma u(x) = f(x)$$

  and boundary conditions (BCs) at $x = a$ and $x = b$

- Standard types of boundary conditions
  - Dirichlet condition: $u(a) = c_1$
  - Neumann condition: $u'(a) = c_1$
  - Robin (or "mixed") condition: $u'(a) + c_2 u(a) = c_3$

Shooting Method

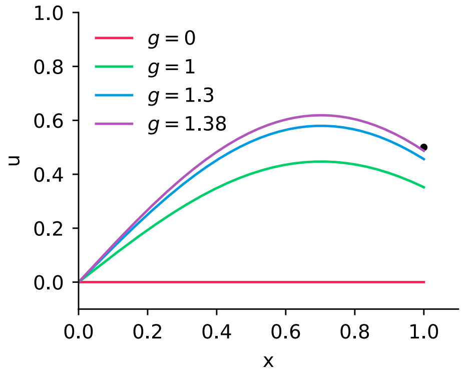
- The shooting method solves the boundary value problem iteratively by solving an initial value problem at each iteration
- To form a correct IVP starting from $x = a$ for a second-order equation, we need two conditions at $x = a$
  - one condition is part of the BVP
  - another condition is imposed with an unknown parameter
- For example, with two Dirichlet conditions $u(a) = c_1$ and $u(b) = c_2$, we can additionally specify $u'(a) = g$
- Solve the IVP, and somehow update g to improve the error $|u(b) - c_2|$
- Not widely used as it relies on nonlinear optimization and does not generalize to PDEs

Shooting Method: Example

- Steady-state diffusion-reaction equation ($\alpha = 1, \gamma = -5$)

$$-\alpha u''(x) + \gamma u(x) = 0, \quad x \in [0, 1]$$

- Dirichlet conditions: $u(0) = 0$ and $u(1) = 0.5$
  and extra Neumann condition: $u(0) = g$
- Iteration: $g_{\text{new}} = g + \eta(0.5 - u(1))$ with $\eta = 2$



- See [examples/unit3/shooting.py]

ODEs: BVP

- A more general approach is to formulate a coupled system of equations for the BVP based on a finite difference approximation
- Suppose we have a grid

$$x_i = a + ih, \quad i = 0, 1, \ldots, n-1$$

  where $h = (b-a)/(n-1)$
- Then our approximation to $u(x)$ is represented by a vector $U \in \mathbb{R}^n$, where $U_i \approx u(x_i)$

ODEs: BVP

- Recall the ODE

$$-\alpha u''(x) + \beta u'(x) + \gamma u(x) = f(x), \quad x \in [a, b]$$

- Let's develop an approximation for each term in the ODE
- For the reaction term γu, we have the pointwise approximation

$$\gamma U_i \approx \gamma u(x_i)$$

ODEs: BVP

- Similarly, for the derivatives
  - Let $D_2 \in \mathbb{R}^{n\times n}$ be the differentiation matrix for the second derivative
  - Let $D_1 \in \mathbb{R}^{n\times n}$ be the differentiation matrix for the first derivative
- Then $-\alpha(D_2U)_i \approx -\alpha u''(x_i)$ and $\beta(D_1U)_i \approx \beta u'(x_i)$
- Hence, we obtain $(AU)_i \approx -\alpha u''(x_i) + \beta u'(x_i) + \gamma u(x_i)$, where $A \in \mathbb{R}^{n\times n}$ is

$$A = -\alpha D_2 + \beta D_1 + \gamma \mathrm{I}$$

- Similarly, we represent the right hand side by sampling f at the grid points, so we introduce $F \in \mathbb{R}^n$, where $F_i = f(x_i)$

ODEs: BVP

- Therefore, we obtain the linear system for $U \in \mathbb{R}^n$

$$AU = F$$

- We have converted a linear differential equation into a linear algebraic equation
- Similarly, we can convert a nonlinear differential equation into a nonlinear algebraic system
- Now we need to account for the boundary conditions

ODEs: BVP

- Dirichlet boundary conditions
  we need to impose $U_0 = c_1$, $U_{n-1} = c_2$
- Since we fix U_0 and U_{n-1}, they are no longer variables:
  we can eliminate them from our linear system
- However, instead of removing rows and columns from A,
  it is more convenient to
  - "zero out" first row of A, then set $A(0, 0) = 1$ and $F_0 = c_1$
  - "zero out" last row of A, then set $A(n-1, n-1) = 1$ and $F_{n-1} = c_2$

ODEs: BVP

- See [examples/unit3/ode_bvp.py]
- Convergence study:

h	**error**
2.0×10^{-2}	5.07×10^{-3}
1.0×10^{-2}	1.26×10^{-3}
5.0×10^{-3}	3.17×10^{-4}
2.5×10^{-3}	7.92×10^{-5}

- $O(h^2)$, as expected due to second-order differentiation matrices

Method of Manufactured Solutions

- The method of manufactured solutions is a technique for testing the implementation
  1. choose a solution u that satisfies the boundary conditions
  2. substitute into the ODE to get a right-hand side f
  3. compute the ODE approximation with f from step 2
  4. verify that you get the expected convergence rate for the approximation to u
- For example, consider $x \in [0,1]$ and set $u(x) = e^x \sin(2\pi x)$

$$\begin{aligned} f(x) &= -\alpha u''(x) + \beta u'(x) + \gamma u(x) \\ &= -\alpha e^x \left[4\pi \cos(2\pi x) + (1-4\pi^2)\sin(2\pi x)\right] + \\ &\quad + \beta e^x \left[\sin(2\pi x) + 2\pi\cos(2\pi x)\right] + \gamma e^x \sin(2\pi x) \end{aligned}$$

Derivatives in BCs

- Question: How would we impose the Robin boundary condition $u'(b) + c_2 u(b) = c_3$, and preserve the $O(h^2)$ convergence rate?
- Option 1: Introduce a ghost node at $x_n = b + h$, this node is involved in both the BC and the $(n-1)$-th matrix row
- Employ central difference approx. to $u'(b)$ to get approx. B.C.:

$$\frac{U_n - U_{n-2}}{2h} + c_2 U_{n-1} = c_3,$$

or equivalently

$$U_n = U_{n-2} - 2hc_2 U_{n-1} + 2hc_3$$

Derivatives in BCs

- The $(n-1)$-th equation is

$$-\alpha\frac{U_{n-2}-2U_{n-1}+U_n}{h^2}+\beta\frac{U_n-U_{n-2}}{2h}+\gamma U_{n-1}=F_{n-1}$$

- We can substitute our expression for U_n into the above equation, and hence eliminate U_n

$$\left(-\frac{2\alpha c_3}{h}+\beta c_3\right)-\frac{2\alpha}{h^2}U_{n-2}+\left(\frac{2\alpha}{h^2}(1+hc_2)-\beta c_2+\gamma\right)U_{n-1}=F_{n-1}$$

- Set $F_{n-1}\leftarrow F_{n-1}-\left(-\frac{2\alpha c_3}{h}+\beta c_3\right)$, we get $n\times n$ system $AU=F$
- Option 2: Use a one-sided finite-difference formula for $u'(b)$ in the Robin BC

Partial Differential Equations

Partial Differential Equations

- As discussed in the introduction, it is a natural extension to consider Partial Differential Equations (PDEs)
- There are three main classes of PDEs:

equation type	**prototypical example**	**equation**
hyperbolic	wave equation	$u_{tt} - u_{xx} = 0$
parabolic	heat equation	$u_t - u_{xx} = f$
elliptic	Poisson equation	$u_{xx} + u_{yy} = f$

- Question: Where do these names come from?

Partial Differential Equations

- Answer: The names are related to conic sections
- General second-order PDEs have the form

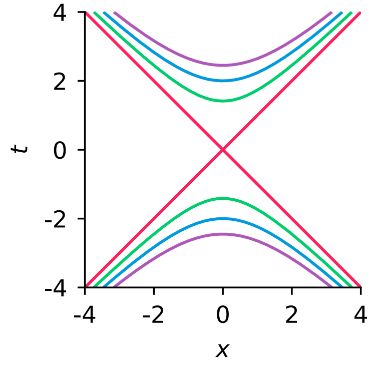
$$au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y + fu + g = 0$$

- This looks like the quadratic function

$$q(x, y) = ax^2 + bxy + cy^2 + dx + ey$$

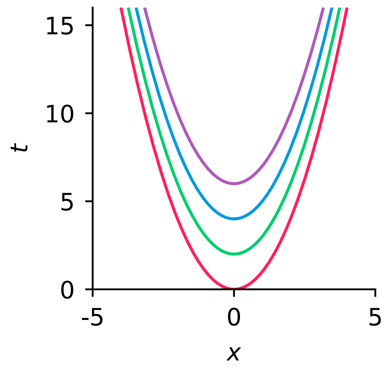
PDEs: Hyperbolic

- Wave equation: $u_{tt} - u_{xx} = 0$
- Corresponding quadratic function is $q(x, t) = t^2 - x^2$
- $q(x, t) = c$ gives a hyperbola, e.g. for $c = 0, 2, 4, 6$, we have



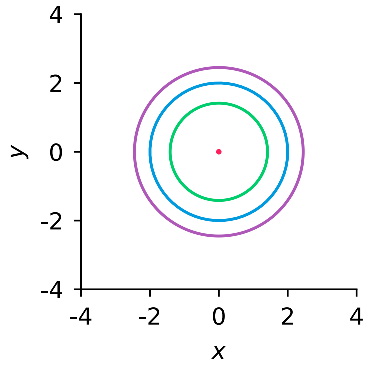
PDEs: Parabolic

- Heat equation: $u_t - u_{xx} = 0$
- Corresponding quadratic function is $q(x, t) = t - x^2$
- $q(x, t) = c$ gives a parabola, e.g. for $c = 0, 2, 4, 6,$ we have



PDEs: Elliptic

- Poisson equation: $u_{xx} + u_{yy} = f$
- Corresponding quadratic function is $q(x, y) = x^2 + y^2$
- $q(x, y) = c$ gives an ellipse, e.g. for $c = 0, 2, 4, 6$, we have



PDEs

- In general, it is not so easy to classify PDEs using conic section naming
- Many problems don't strictly fit into the classification scheme
  (e.g. nonlinear, or higher order, or variable coefficient equations)
- Nevertheless, the names hyperbolic, parabolic, elliptic are the standard ways of describing PDEs, based on the criteria:
  - Hyperbolic: time-dependent, conservative physical process,
    no steady state
  - Parabolic: time-dependent, dissipative physical process,
    evolves towards steady state
  - Elliptic: describes systems at equilibrium/steady-state

Hyperbolic PDEs

- We introduced the wave equation $u_{tt} - u_{xx} = 0$ above
- Note that the system of first order PDEs

$$u_t + v_x = 0$$
$$v_t + u_x = 0$$

  is equivalent to the wave equation, since

$$u_{tt} = (u_t)_t = (-v_x)_t = -(v_t)_x = -(-u_x)_x = u_{xx}$$

- This assumes that u, v are smooth,
  so we can switch the order of the partial derivatives

Hyperbolic PDEs

- Hence we will focus on the linear advection equation

$$u_t + cu_x = 0$$

  with initial condition $u(x,0) = u_0(x)$, and $c \in \mathbb{R}$
- This equation is representative of hyperbolic PDEs in general
- This is a first order PDE and does not correspond to a conic section
- However, it is still considered hyperbolic since it is
  - time-dependent
  - conservative
  - not evolving toward steady state

Hyperbolic PDEs

- We can see that $u(x,t) = u_0(x - ct)$ satisfies the PDE
- Let $z(x,t) = x - ct$, then from the chain rule we have

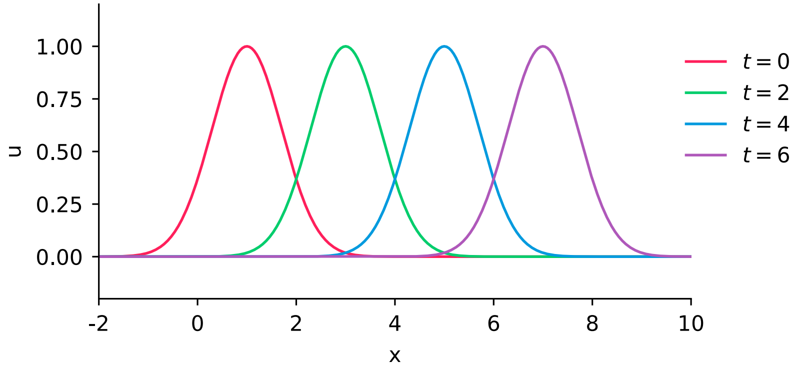
$$\begin{aligned}
\frac{\partial}{\partial t} u_0(x - ct) + c\frac{\partial}{\partial x} u_0(x - ct) &= \frac{\partial}{\partial t} u_0(z(x,t)) + c\frac{\partial}{\partial x} u_0(z(x,t)) \\
&= u_0'(z)\frac{\partial z}{\partial t} + c u_0'(z)\frac{\partial z}{\partial x} \\
&= -c u_0'(z) + c u_0'(z) \\
&= 0
\end{aligned}$$

Hyperbolic PDEs

- This tells us that the equation transports (or advects) the initial condition with "speed" c

$$u_t + cu_x = 0$$

- For example, with $c = 1$ and an initial condition $u_0(x) = e^{-(1-x)^2}$



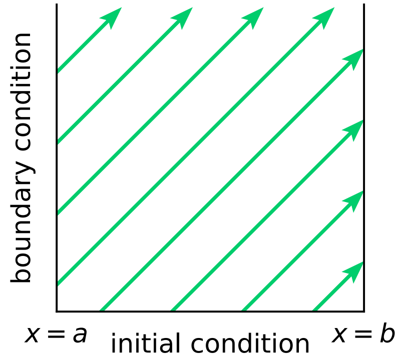
Characteristics

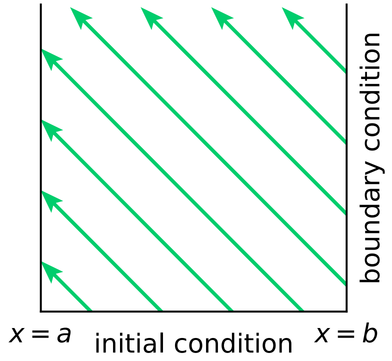
- We can understand the behavior of hyperbolic PDEs in more detail by considering characteristics
- Characteristics are paths $(X(t), t)$ in the xt-plane on which the solution is constant
- For $u_t + cu_x = 0$ we have $X(t) = X_0 + ct$, since

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} u(X(t), t) &= u_t(X(t), t) + u_x(X(t), t)\frac{\mathrm{d}X(t)}{\mathrm{d}t} \\ &= u_t(X(t), t) + cu_x(X(t), t) \\ &= 0\end{aligned}$$

Characteristics

- Hence $u(X(t),t) = u(X(0),0) = u_0(X_0)$, i.e. the initial condition is transported along characteristics
- Characteristics have important implications for the direction of flow of information, and for boundary conditions





$c > 0$, must impose BC at $x = a$
cannot impose BC at $x = b$

$c < 0$, must impose BC at $x = b$
cannot impose BC at $x = a$

Characteristics

- More generally, if we have a non-zero right-hand side in the PDE, then the situation is a bit more complicated on each characteristic
- Consider $u_t + cu_x = f(t, x, u(t, x))$, and $X(t) = X_0 + ct$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}u(X(t), t) &= u_t(X(t), t) + u_x(X(t), t)\frac{\mathrm{d}X(t)}{\mathrm{d}t} \\ &= u_t(X(t), t) + cu_x(X(t), t) \\ &= f(t, X(t), u(X(t), t))\end{aligned}$$

- In this case, the solution is no longer constant on $(X(t), t)$, but we have reduced a PDE to a set of ODEs, so that

$$u(X(t), t) = u_0(X_0) + \int_0^t f(t, X(t), u(X(t), t)\mathrm{d}t$$

Characteristics

- We can also find characteristics for advection with a variable coefficient
- Exercise: Verify that the characteristic curve for

$$u_t + c(t, x)u_x = 0$$

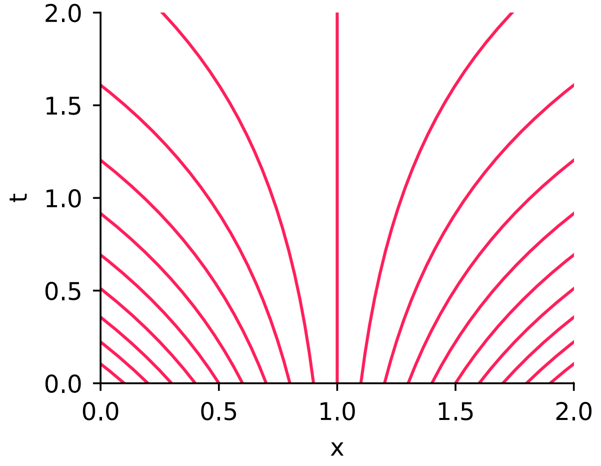
is given by

$$X'(t) = c(X(t), t)$$

- In this case, we have to solve an ODE to obtain the curve $(X(t), t)$ in the xt-plane

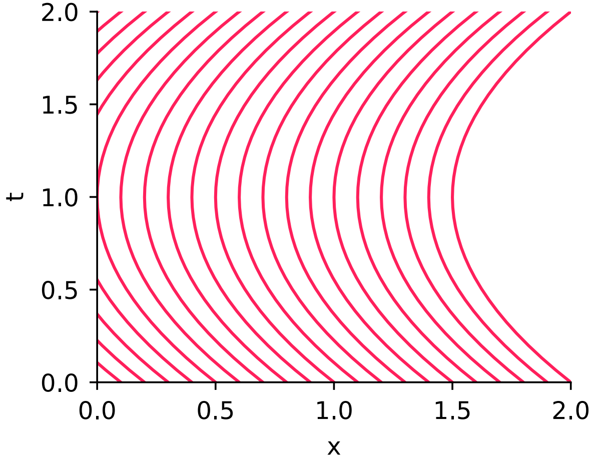
Example: Variable Speed in Space

- Equation: $u_t + cu_x = 0$ with $c(x,t) = x - 1$
- Characteristics satisfy $X'(t) = c(X(t), t)$ with solution $X(t) = 1 + (X_0 - 1)e^t$
- Characteristics "bend away" from $x = 1$



Example: Variable Speed in Time

- Equation: $u_t + cu_x = 0$ with $c(x,t) = t - 1$
- Characteristics satisfy $X'(t) = c(X(t), t)$ with solution $X(t) = X_0 + \frac{1}{2}t^2 - t$
- The same shape shifted along x

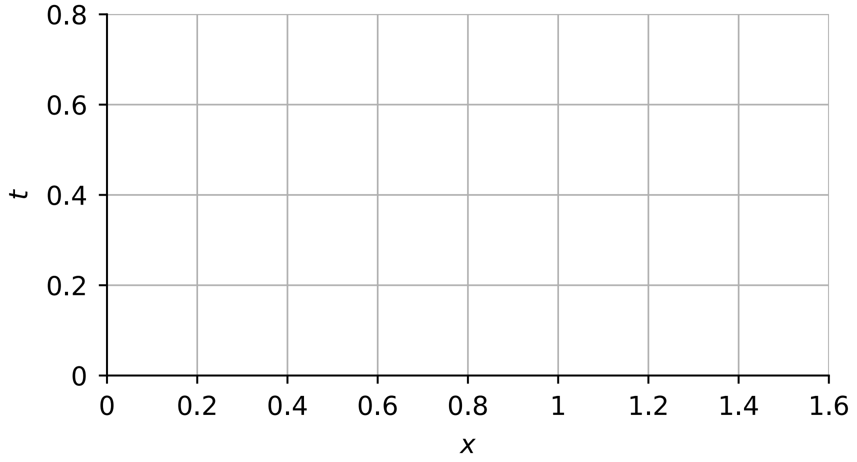


Hyperbolic PDEs: Numerical Approximation

- We now consider how to solve
$$u_t + cu_x = 0$$
using a finite difference method
- Question: Why finite differences? Why not just use characteristics?
- Answer: Characteristics actually are a viable option for computational methods, and are used in practice
- However, characteristic methods can become very complicated in 2D or 3D, or for nonlinear problems
- Finite differences are a much more practical choice

Hyperbolic PDEs: Numerical Approximation

- We impose an initial condition and a boundary condition
- A finite difference approximation is performed on a grid in the xt-plane



Hyperbolic PDEs: Numerical Approximation

- The first step in developing a finite difference approximation is to consider the Courant–Friedrichs–Lewy (CFL) condition
- The CFL condition is a necessary condition for the convergence of a finite difference approximation of a hyperbolic problem
- Suppose we discretize $u_t + cu_x = 0$ in space and time using the explicit scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + c\frac{U_j^n - U_{j-1}^n}{\Delta x} = 0$$

- Here $U_j^n \approx u(t_n, x_j)$, where $t_n = n\Delta t$, $x_j = j\Delta x$

Hyperbolic PDEs: Numerical Approximation

- This can be rewritten as

$$\begin{aligned} U_j^{n+1} &= U_j^n - \frac{c\Delta t}{\Delta x}(U_j^n - U_{j-1}^n) \\ &= (1-\nu)U_j^n + \nu U_{j-1}^n \end{aligned}$$

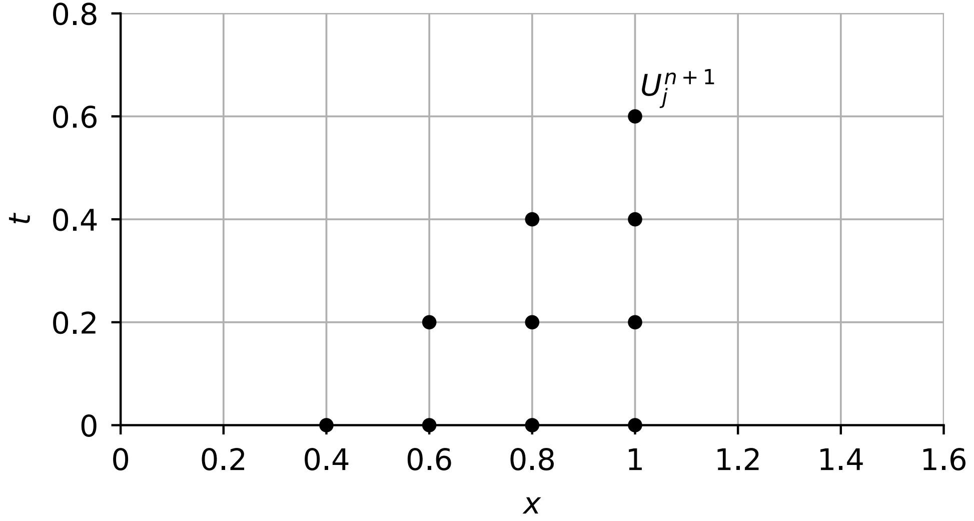
  where

$$\nu = \frac{c\Delta t}{\Delta x}$$

- We can see that U_j^{n+1} depends only on U_j^n and U_{j-1}^n

Hyperbolic PDEs: Numerical Approximation

- The set of grid nodes on which U_j^{n+1} depends is called the domain of dependence of U_j^{n+1}



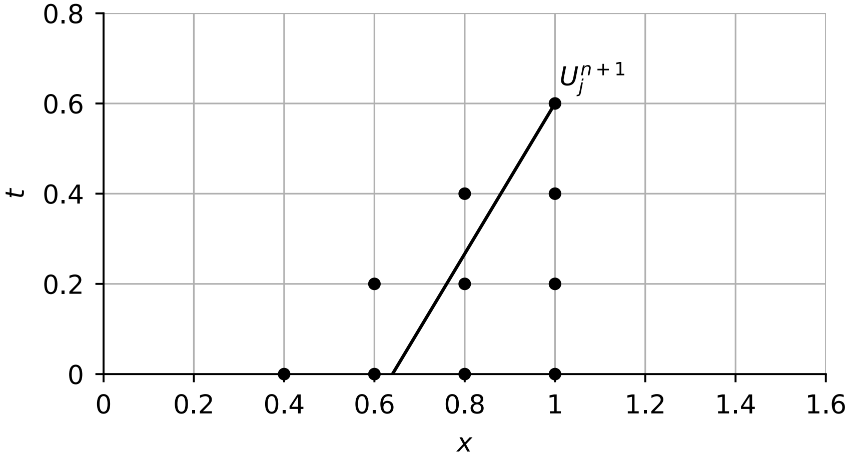
Hyperbolic PDEs: Numerical Approximation

- The domain of dependence of the exact solution $u(t_{n+1}, x_j)$ is determined by the characteristics passing through (t_{n+1}, x_j)
- The CFL condition states

  For a convergent scheme, the domain of dependence of the PDE must lie within the domain of dependence of the numerical method

Hyperbolic PDEs: Numerical Approximation

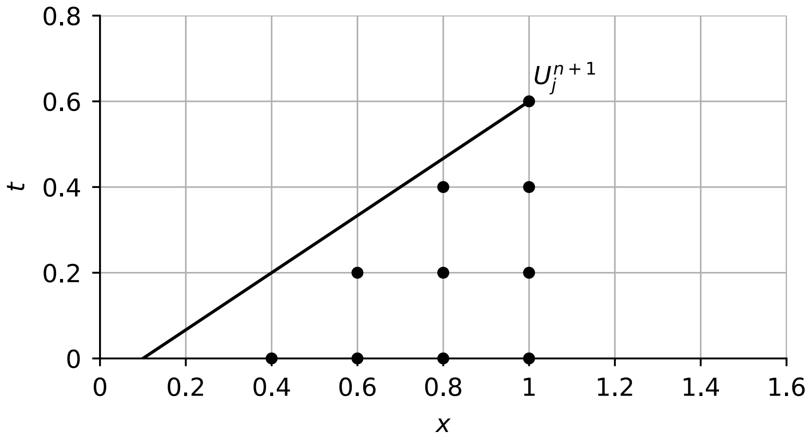
- Domain of dependence of U_j^n: grid nodes •
- Domain of dependence of $u(t_{n+1}, x_j)$: solid line (characteristic)



- In this case, the scheme satisfies the CFL condition

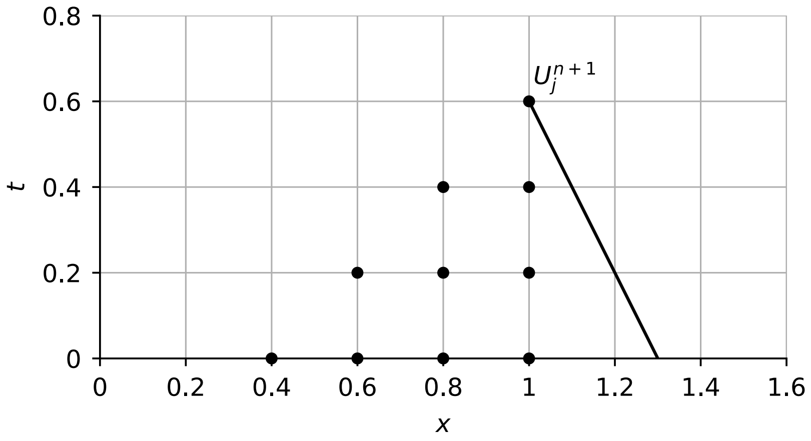
Hyperbolic PDEs: Numerical Approximation

- With a larger advection speed c,
  the scheme does not satisfy the CFL condition



Hyperbolic PDEs: Numerical Approximation

- With a negative advection speed ($c < 0$), the scheme does not satisfy the CFL condition

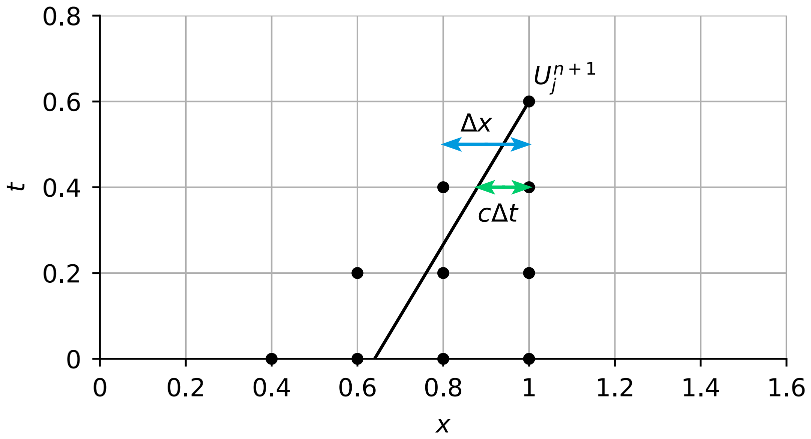


Hyperbolic PDEs: Numerical Approximation

- Question: What goes wrong if the CFL condition is violated?
- Answer: The exact solution $u(x, t)$ depends on initial value $u_0(x_0)$, which is outside the scheme's domain of dependence
- Therefore, the numerical approximation to $u(x, t)$ is "insensitive" to the value $u_0(x_0)$, which means that the method cannot be convergent

Hyperbolic PDEs: Numerical Approximation

- If $c > 0$, then we require $\nu = \frac{c\Delta t}{\Delta x} \leq 1$ for the CFL condition to be satisfied



Hyperbolic PDEs: Numerical Approximation

- Note that CFL is only a necessary condition for convergence
- However, CFL is straightforward to test and allows us to easily reject improper schemes or parameters
- For example, for $u_t + cu_x = 0$, the scheme with a backward difference

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + c\frac{U_j^n - U_{j-1}^n}{\Delta x} = 0$$

  cannot be convergent if $c < 0$
- Question: How should we modify the scheme for $c < 0$?

Hyperbolic PDEs: Upwind Method

- Answer: The method should account for the direction of "information flow"
- This motivates the upwind scheme for $u_t + cu_x = 0$

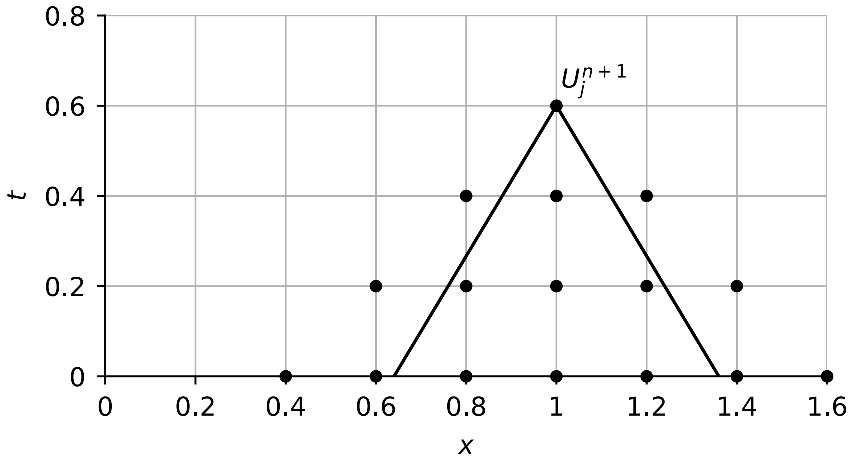
$$U_j^{n+1} = \begin{cases} U_j^n - c\frac{\Delta t}{\Delta x}(U_j^n - U_{j-1}^n), & \text{if } c > 0 \\ U_j^n - c\frac{\Delta t}{\Delta x}(U_{j+1}^n - U_j^n), & \text{if } c < 0 \end{cases}$$

- The upwind scheme satisfies CFL condition if $|\nu| = |c\Delta t/\Delta x| \leq 1$
- $\nu = c\Delta t/\Delta x$ is called the CFL number (or the Courant number)

Hyperbolic PDEs: Central Difference

- Another method that seems appealing is the central difference method

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + c\frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x} = 0$$



- It satisfies CFL for $|\nu| = |c\Delta t/\Delta x| \leq 1$ both for $c > 0$ and $c < 0$
- However, we will see that this method is unstable

Hyperbolic PDEs: Accuracy

- Recall that truncation error is
  the residual of the numerical approximation
  evaluated on the exact solution
- For the $(c > 0)$ upwind method, the truncation error is:

$$T_j^n = \frac{u(t^{n+1}, x_j) - u(t^n, x_j)}{\Delta t} + c\frac{u(t^n, x_j) - u(t^n, x_{j-1})}{\Delta x}$$

- The order of accuracy is then the largest p such that

$$T_j^n = \mathcal{O}((\Delta x)^p + (\Delta t)^p)$$

Hyperbolic PDEs: Accuracy

- For the upwind method, we have

$$T_j^n = \frac{1}{2}\left[\Delta t\, u_{tt}(t^n, x_j) - c\Delta x\, u_{xx}(t^n, x_j)\right] + \text{h.o.t.}$$

- Hence the upwind scheme is first order accurate

Hyperbolic PDEs: Accuracy

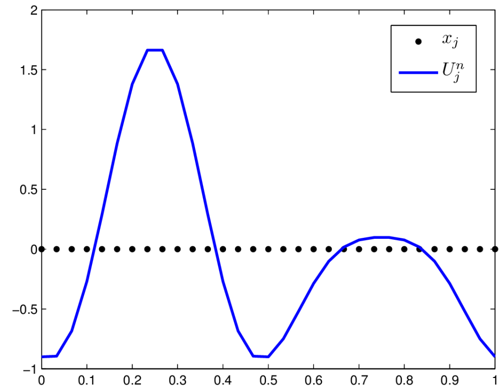
- Just like with ODEs, truncation error is related to convergence to the exact solution as $\Delta t, \Delta x \to 0$
- Note that to let $\Delta t, \Delta x \to 0$, we generally need to decide on a relationship between Δt and Δx
- For example, to let $\Delta t, \Delta x \to 0$ for the upwind scheme, we would set $\frac{c\Delta t}{\Delta x} = \nu \in (0, 1]$.
  This ensures CFL is satisfied for all $\Delta x, \Delta t$

Hyperbolic PDEs: Accuracy

- In general, convergence of a finite difference method for a PDE is related to both its truncation error and its stability
- Now we will consider how to analyze stability using the Fourier stability analysis (also called von Neumann analysis)

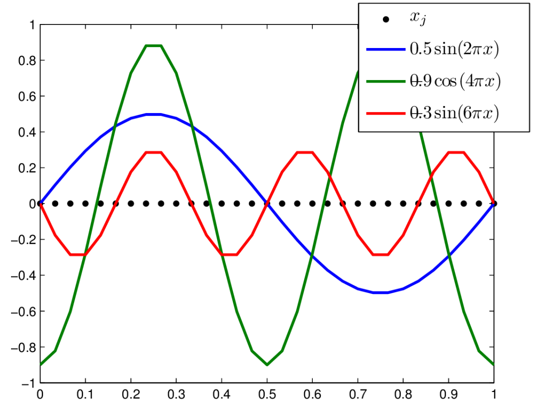
Hyperbolic PDEs: Stability

- Suppose that U_j^n is periodic on a grid $x_1, x_2, \ldots, x_n$



Hyperbolic PDEs: Stability

- Then we can represent U_j^n as a linear combination of sin and cos functions, i.e. Fourier modes



- Equivalently, as a linear combination of complex exponentials, since $e^{ikx} = \cos(kx) + i\sin(kx)$ so that

$$\sin(x) = \frac{1}{2i}(e^{ix} - e^{-ix}), \qquad \cos(x) = \frac{1}{2}(e^{ix} + e^{-ix})$$

Hyperbolic PDEs: Stability

- Let's focus on only one of the Fourier modes
- In particular, we consider the ansatz $U_j^n(k) = \lambda(k)^n e^{ikx_j}$, where k is the wave number and $\lambda(k) \in \mathbb{C}$
- Key idea: Suppose that $U_j^n(k)$ satisfies our finite difference equation, then this will allow us to solve for $\lambda(k)$
- The value of $|\lambda(k)|$ indicates whether the Fourier mode e^{ikx_j} is amplified or damped
- If $|\lambda(k)| \leq 1$ for all k then the scheme does not amplify any Fourier modes, therefore is stable

Hyperbolic PDEs: Stability

- We now perform Fourier stability analysis for the upwind scheme with $c > 0$ (recall that $\nu = \frac{c\Delta t}{\Delta x}$):

$$U_j^{n+1} = U_j^n - \nu(U_j^n - U_{j-1}^n)$$

- Substituting in $U_j^n(k) = \lambda(k)^n e^{ik(j\Delta x)}$ gives

$$\begin{aligned} \lambda(k)e^{ik(j\Delta x)} &= e^{ik(j\Delta x)} - \nu(e^{ik(j\Delta x)} - e^{ik((j-1)\Delta x)}) \\ &= e^{ik(j\Delta x)} - \nu e^{ik(j\Delta x)}(1 - e^{-ik\Delta x}) \end{aligned}$$

- Then

$$\lambda(k) = 1 - \nu(1 - e^{-ik\Delta x}) = 1 - \nu(1 - \cos(k\Delta x) + i\sin(k\Delta x))$$

Hyperbolic PDEs: Stability

- It follows that

$$\begin{aligned}|\lambda(k)|^2 &= [(1-\nu)+\nu\cos(k\Delta x)]^2 + [\nu\sin(k\Delta x)]^2 \\ &= (1-\nu)^2+\nu^2+2\nu(1-\nu)\cos(k\Delta x) \\ &= 1-2\nu(1-\nu)(1-\cos(k\Delta x))\end{aligned}$$

and from the identity $(1-\cos(\theta)) = 2\sin^2(\frac{\theta}{2})$, we have

$$|\lambda(k)|^2 = 1 - 4\nu(1-\nu)\sin^2\left(\frac{1}{2}k\Delta x\right)$$

- Due to the CFL condition, we first suppose that $0 \leq \nu \leq 1$
- Then $0 \leq 4\nu(1-\nu)\sin^2\left(\frac{1}{2}k\Delta x\right) \leq 1$, and therefore $|\lambda(k)| \leq 1$

Hyperbolic PDEs: Stability

- In contrast, consider stability of the central difference scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + c\frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x} = 0$$

- Recall that this also satisfies the CFL condition as long as $|\nu| \leq 1$
- But Fourier stability analysis yields

$$\lambda(k) = 1 - \nu i \sin(k\Delta x) \implies |\lambda(k)|^2 = 1 + \nu^2 \sin^2(k\Delta x)$$

and hence $|\lambda(k)| > 1$ (unless $\sin(k\Delta x) = 0$), i.e. unstable!

Consistency

- We say that a numerical scheme is consistent with a PDE if its truncation error tends to zero as $\Delta x, \Delta t \to 0$
- For example, any first (or higher) order scheme is consistent

Lax Equivalence Theorem

- Then a fundamental theorem about finite difference schemes is the Lax equivalence theorem

  For a consistent finite difference approximation to a linear evolutionary problem, the stability of the scheme is necessary and sufficient for convergence

- This theorem refers to linear evolutionary problems, e.g. linear hyperbolic or parabolic PDEs
- Due to Peter Lax (born 1926, American mathematician)

Lax Equivalence Theorem

- We know how to check consistency: Derive the truncation error
- We know how to check stability: Fourier stability analysis
- Hence, from the Lax equivalence theorem,
  we have a general approach for verifying convergence
- Also, as with ODEs, convergence rate is determined by truncation error

Lax Equivalence Theorem

- Note that strictly speaking Fourier stability analysis only applies for periodic problems
- However, its conclusions on periodic problems generally hold in other cases
- Fourier stability analysis is the standard tool for examining stability of finite-difference methods for PDEs
- See [examples/unit3/advection.py], one-sided and central difference schemes for the advection equation

Hyperbolic PDEs: Semi-discretization

- So far, we have developed full discretizations (both space and time) of the advection equation, and considered accuracy and stability
- However, it can be helpful to consider semi-discretizations, where we discretize only in space, or only in time
- For example, discretizing $u_t + c(t,x)u_x = 0$ in space using a backward difference formula gives

$$\frac{\partial U_j(t)}{\partial t} + c_j(t)\frac{U_j(t) - U_{j-1}(t)}{\Delta x} = 0, \qquad j = 1, \ldots, n$$

Hyperbolic PDEs: Semi-discretization

- This gives a system of ODEs, $U_t = f(t, U(t))$, where $U(t) \in \mathbb{R}^n$ and

$$f_j(t, U(t)) = -c_j(t) \frac{U_j(t) - U_{j-1}(t)}{\Delta x}$$

- Forward Euler applied to that system yields the first-order upwind scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = f(t^n, U^n) = -c_j^n \frac{U_j^n - U_{j-1}^n}{\Delta x}$$

- Backward Euler yields the implicit first-order upwind

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = f(t^{n+1}, U^{n+1}) = -c_j^{n+1} \frac{U_j^{n+1} - U_{j-1}^{n+1}}{\Delta x}$$

Hyperbolic PDEs: Method of Lines

- We can also use a "black box" ODE solver (e.g. `scipy.integrate.odeint`) to solve the system of ODEs
- This "black box" approach is called the method of lines
- The name "lines" is because we solve each $U_j(t)$ for a fixed x_j, i.e. a line in the xt-plane
- We let the ODE solver to choose step size Δt to obtain a stable and accurate scheme

Wave Equation

- We now briefly return to the wave equation:

$$u_{tt} - c^2 u_{xx} = 0$$

- In one spatial dimension, this models vibrations of a string

Wave Equation

- Many schemes have been proposed for the wave equation, as well as other hyperbolic systems in general
- One good option is to use central difference approximations for both u_{tt} and u_{xx}

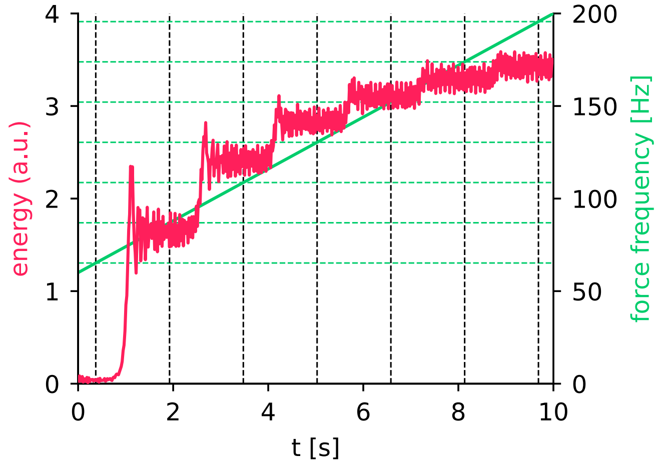
$$\frac{U_j^{n+1} - 2U_j^n + U_j^{n-1}}{\Delta t^2} - c^2 \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{\Delta x^2} = 0$$

- Key points
  - truncation error analysis $\implies$ second-order accurate
  - Fourier stability analysis $\implies$ stable for $0 \leq c\Delta t/\Delta x \leq 1$
  - two-step method in time, need a one-step method to "get started"
- See [examples/unit3/wave.py] and [examples/unit3/wave_audio.py]

Wave Equation: Example

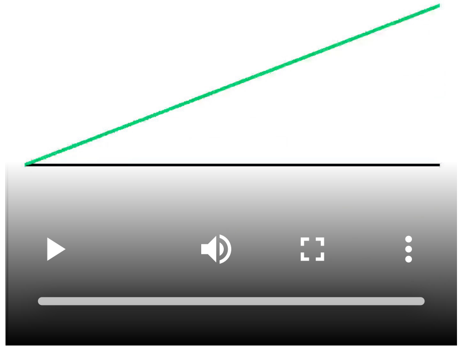
- Wave equation with forcing

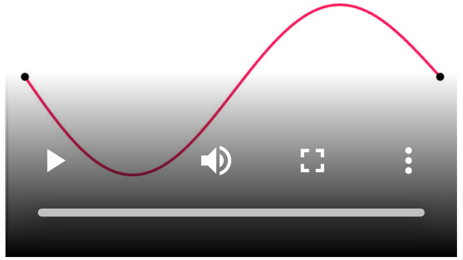
$$u_{tt} - u_{xx} = f$$



- Energy $\int u_t^2 dx$
- Sound $\int u_x^2 dx$ (change in arc length)

- Forcing $f = x \sin(\omega(t)t)$
  $\omega(t) = at + b$





Heat Equation

- The canonical parabolic equation is the heat equation

$$u_t - \alpha u_{xx} = f(t,x)$$

  where α is the thermal diffusivity
- By rescaling x and t, we can assume $\alpha = 1$
- To form an initial-boundary value problem, we impose
  - initial condition $u(0,x) = u_0(x)$
  - boundary conditions on both endpoints the domain

Heat Equation

- A natural idea would be to discretize u_{xx} with a central difference, and employ forward Euler in time

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} - \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{\Delta x^2} = 0$$

- Or we could use backward Euler in time

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} - \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{\Delta x^2} = 0$$

Heat Equation

- Or we could do the midpoint rule in time

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} - \frac{1}{2}\frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{\Delta x^2} - \frac{1}{2}\frac{U_{j-1}^{n} - 2U_j^{n} + U_{j+1}^{n}}{\Delta x^2} = 0$$

- This is called the Crank–Nicolson method
- Extra reading: Crank & Nicolson, 1947. A practical method for numerical evaluation of solutions of partial differential equations of the heat-conduction type

θ-Method

- The θ-method is a family of methods that includes all of the above

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} - \theta \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{\Delta x^2} - (1-\theta)\frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{\Delta x^2} = 0$$

  where $\theta \in [0,1]$ is a parameter
  - $\theta = 0 \implies$ forward Euler
  - $\theta = \frac{1}{2} \implies$ Crank–Nicolson
  - $\theta = 1 \implies$ backward Euler
- For the θ-method, we can
  - perform Fourier stability analysis
  - calculate the truncation error

θ-Method: Stability

- Fourier stability analysis. Set $U_j^n(k) = \lambda(k)^n e^{ik(j\Delta x)}$ to get

$$\lambda(k) = \frac{1 - 4(1-\theta)\mu \sin^2\left(\frac{1}{2}k\Delta x\right)}{1 + 4\theta\mu \sin^2\left(\frac{1}{2}k\Delta x\right)}$$

  where $\mu = \Delta t/\Delta x^2$

- In general, $\mu = \alpha\Delta t/\Delta x^2$ is dimensionless (sometimes called the diffusion number, or diffusion CFL number)
- Here we cannot get $\lambda(k) > 1$, hence only concern is $\lambda(k) < -1$
- Let's find conditions for stability, i.e. we want $\lambda(k) \geq -1$

$$1 - 4(1-\theta)\mu \sin^2\left(\frac{1}{2}k\Delta x\right) \geq -\left[1 + 4\theta\mu \sin^2\left(\frac{1}{2}k\Delta x\right)\right]$$

θ-Method: Stability

- Or equivalently

$$4\mu(1-2\theta)\sin^2\left(\frac{1}{2}k\Delta x\right) \le 2$$

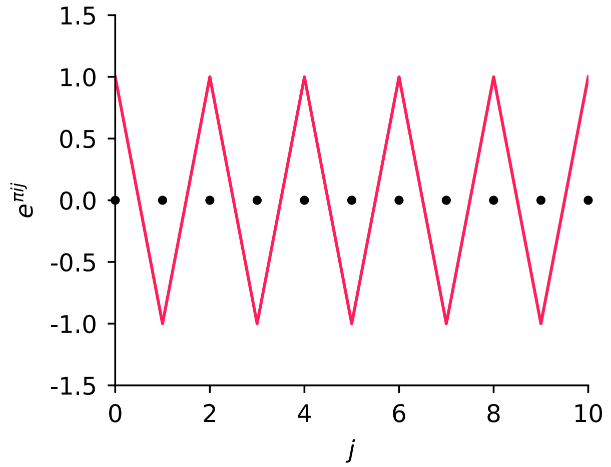
- For $\theta \in [0.5, 1]$ this inequality is always satisfied, hence the θ-method is unconditionally stable (i.e. stable independent of μ)
- For $\theta \in [0, 0.5)$, the "most unstable" Fourier mode is at $k = \pi/\Delta x$, since this maximizes the factor $\sin^2\left(\frac{1}{2}k\Delta x\right)$

θ-Method: Stability

- Note that this corresponds to the highest frequency mode that can be represented on our grid, since with $k = \pi/\Delta x$ we have

$$e^{ik(j\Delta x)} = e^{\pi i j} = (e^{\pi i})^j = (-1)^j$$

- The $k = \pi/\Delta x$ "sawtooth" mode



θ-Method: Stability

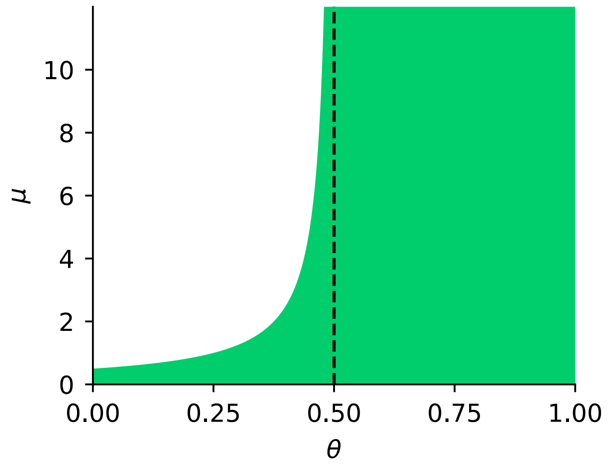
- This sawtooth mode is stable (and so all modes are stable) if

$$4\mu(1-2\theta) \leq 2 \iff \mu \leq \frac{1}{2(1-2\theta)}$$

- Therefore, the θ-method is conditionally stable for $\theta \in [0, 0.5)$

θ-Method: Stability

- The θ-method is conditionally stable if $\theta \in [0, 0.5)$ and unconditionally stable if $\theta \in [0.5, 1]$
- Stability region in the μ-θ plane



θ-Method: Stability

- Note that θ in $[0, 0.5)$ leads to a severe stability restriction, since Δt is quadratic in Δx

$$\Delta t \leq \frac{(\Delta x)^2}{2(1-2\theta)}$$

- Recall that in the hyperbolic case, Δt is linear in Δx

$$\Delta t \leq \frac{\Delta x}{c}$$

- This indicates that spacial discretization of the heat equation results in a stiff system of ODEs

θ-Method: Accuracy

- The truncation error analysis gives

$$
\begin{aligned}
T_j^n &= \frac{u_j^{n+1} - u_j^n}{\Delta t} - \theta \frac{u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}}{\Delta x^2} - (1-\theta)\frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{\Delta x^2} \\
&= [u_t - u_{xx}] + \left[\left(\tfrac{1}{2} - \theta\right)\Delta t u_{xxt} - \tfrac{1}{12}\Delta x^2 u_{xxxx}\right] \\
&\qquad + \left[\tfrac{1}{24}\Delta t^2 u_{ttt} - \tfrac{1}{8}\Delta t^2 u_{xxtt}\right] \\
&\qquad + \left[\tfrac{1}{12}\left(\tfrac{1}{2} - \theta\right)\Delta t \Delta x^2 u_{xxxxt} - \tfrac{2}{6!}\Delta x^4 u_{xxxxxx}\right] + \cdots
\end{aligned}
$$

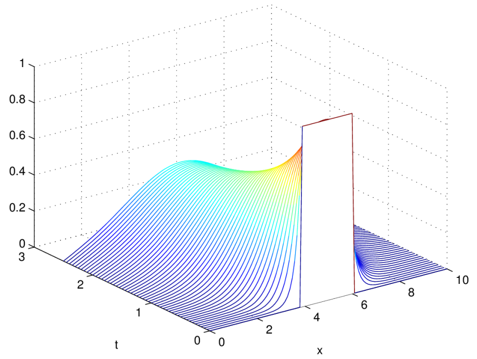
- The term $u_t - u_{xx}$ in T_j^n vanishes since u solves the PDE

θ-Method: Accuracy

- The method is second order if $\theta = 0.5$, and first order otherwise if $\theta \neq 0.5$
- The θ-method is consistent (i.e. truncation error tends to zero) and stable (conditionally stable for $\theta \in [0, 0.5)$)
- Therefore, from the Lax equivalence theorem, the method is convergent

Heat Equation

- Note that the heat equation describes a diffusive process, so it tends to smooth out discontinuities
- See [examples/unit3/heat.py], forward Euler and Crank-Nicolson schemes for the heat equation



- This is qualitatively different to hyperbolic equations, e.g. the advection equation will just transport a discontinuity in u_0

Elliptic PDEs

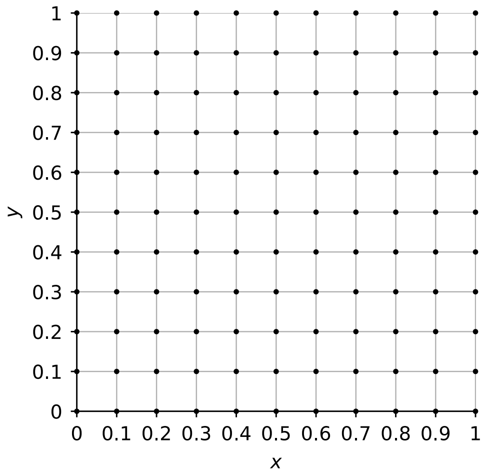
- The canonical elliptic PDE is the Poisson equation

$$u_{xx} + u_{yy} = f(x, y)$$

  for $(x, y) \in \Omega$ in the domain $\Omega \subset \mathbb{R}^2$
- This is generally written as $\nabla^2 u = f$ (or $\Delta u = f$)
- Options for boundary conditions on the domain boundary $\partial\Omega$
  - Dirichlet, given value u
  - Neumann, given normal derivative $\frac{\partial u}{\partial n}$
  - Robin (mixed), given linear combination of both

Elliptic PDEs

- We will consider how to use a finite difference scheme to approximate this 2D Poisson equation
- First, introduce a uniform grid to discretize Ω



Elliptic PDEs

- Assume equal grid spacing $h = \Delta x = \Delta y$
- Then
  - $x_i = ih, i = 0, 1, 2 \ldots, N_x - 1,$
  - $y_j = jh, j = 0, 1, 2, \ldots, N_y - 1,$
  - $U_{i,j} \approx u(x_i, y_j)$
- Use finite differences to approximate u_{xx} and u_{yy} on this grid

Elliptic PDEs

- Each derivative is approximated as

$$u_{xx}(x_i, y_j) = \frac{u(x_{i-1}, y_j) - 2u(x_i, y_j) + u(x_{i+1}, y_j)}{h^2} + O(h^2)$$

$$u_{yy}(x_i, y_j) = \frac{u(x_i, y_{j-1}) - 2u(x_i, y_j) + u(x_i, y_{j+1})}{h^2} + O(h^2)$$

- The Laplacian is approximated as

$$u_{xx}(x_i, y_j) + u_{yy}(x_i, y_j) =$$

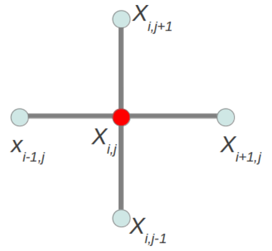
$$\frac{u(x_i, y_{j-1}) + u(x_{i-1}, y_j) - 4u(x_i, y_j) + u(x_{i+1}, y_j) + u(x_i, y_{j+1})}{h^2} + O(h^2)$$

Elliptic PDEs

- Using the grid values, the approximation to the Laplacian is

$$u_{xx} + u_{yy} \approx \frac{U_{i,j-1} + U_{i-1,j} - 4U_{i,j} + U_{i+1,j} + U_{i,j+1}}{h^2}$$

- This corresponds to a 5-point stencil

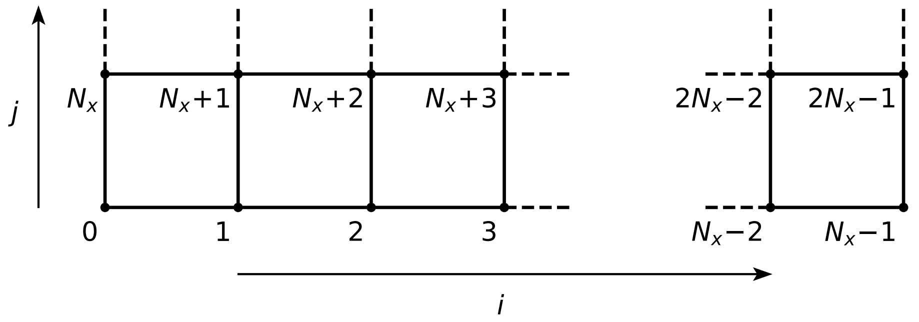


Elliptic PDEs

- We represent the numerical solution as a vector $U \in \mathbb{R}^{N_x N_y}$
- We want to construct a differentiation matrix $D \in \mathbb{R}^{N_x N_y \times N_x N_y}$ that approximates the Laplacian
- Question: How many non-zero diagonals will D have?
- To construct D, we need to relate the entries of the one-dimensional vector U to the two-dimensional grid values $U_{i,j}$ (i.e. flatten the grid values)

Elliptic PDEs

- For instance, let's enumerate the nodes from 0 to $N_x N_y - 1$ starting from the bottom row $j = 0$ (i.e. row-major order)



- Let G denote the mapping from the 2D indexing to the 1D indexing
- From the above schematic we have

$$G(i,j) = jN_x + i \quad \text{and therefore} \quad U_{G(i,j)} = U_{i,j}$$

Elliptic PDEs

- Let's focus on node (i, j), this corresponds to entry $G(i, j)$ of U
- Due to the 5-point stencil, row $G(i, j)$ of D will only have non-zeros in five columns with indices

$$\begin{aligned} G(i, j-1) &= G(i, j) - N_x \\ G(i-1, j) &= G(i, j) - 1 \\ G(i, j) &= G(i, j) \\ G(i+1, j) &= G(i, j) + 1 \\ G(i, j+1) &= G(i, j) + N_x \end{aligned}$$

Elliptic PDEs

- The discretization of the equations above applies in inner nodes, i.e. nodes with indices

$$i > 0, \quad i < N_x - 1, \quad j > 0, \quad \text{and} \quad j < N_y - 1$$

- Impose zero Dirichlet conditions

$$U_{i,j} = 0$$

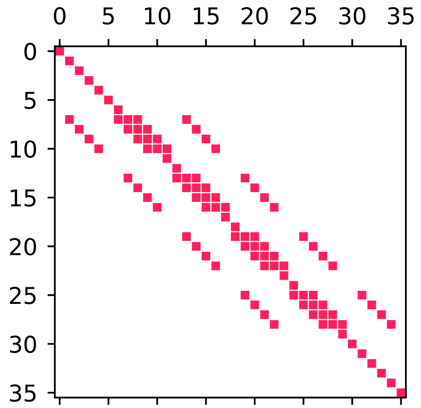
  on the boundaries, i.e. nodes with indices

$$i = 0, \quad i = N_x - 1, \quad j = 0, \quad \text{or} \quad j = N_y - 1$$

- Other cases (e.g. Neumann conditions) will need to be discretized accordingly on each boundary

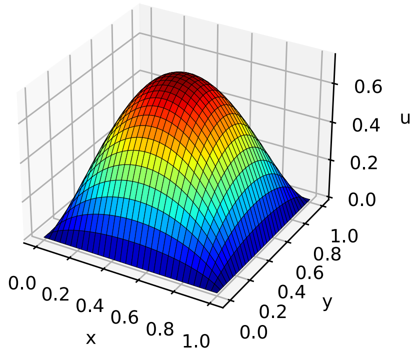
Elliptic PDEs

- For example, in the case $N_x = N_y = 6$, matrix D has the following sparsity pattern



Elliptic PDEs

- Poisson equation $\nabla^2 u = -10$
  for $(x, y) \in \Omega = [0, 1]^2$ with $u = 0$ on $\partial\Omega$



- See [examples/unit3/poisson.py], solved using `scipy.sparse`