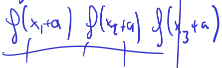
Announcements

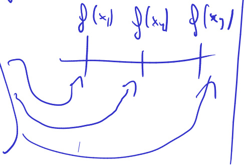
- ICES
- Final
- 4CH2: no penalty
  if turned in by Dec 12
- Exam 3 page grades out

Review

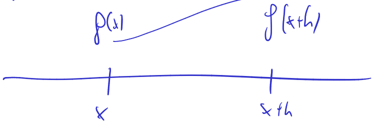


$$D = V' V^{-1}$$

$$D = \begin{bmatrix} o & o & o \\ o & o & o \\ o & o & o \end{bmatrix}$$



$$\alpha f(x+h) + \beta f(x) = \frac{f(x+h) - f(x)}{h} \approx f'(x)$$

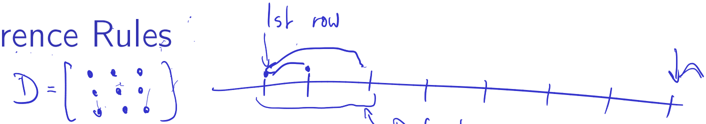


Goals

- Noise and differentiation
- Richardson extrapolation
- IVP

More Finite Difference Rules

Similarly:



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

D for these three nodes

(Centered differences)

Can also take higher order derivatives:

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

Can find these by trying to match Taylor terms.
Alternative: Use linear algebra with interpolate-then-differentiate to find FD formulas.

Demo: Finite Differences vs Noise [cleared]

Demo: Floating point vs Finite Differences [cleared]

Richardson Extrapolation

Deriving high-order methods is hard work. Can I just do multiple low-order approximations (with different h and get a high-order one out?

Suppose we have $F = \tilde{F}(h) + O(h^p)$ and $\tilde{F}(h_1)$ *and* $\tilde{F}(h_2)$.

$$\tilde{F}(h_1) \quad \tilde{F}(h_2)$$

$$F = \tilde{F}(h) + a h^p + O(h^q)$$

$$F = \alpha \tilde{F}(h_1) + \beta \tilde{F}(h_2) + O(h^q)$$

$$\alpha + \beta = 1$$

$$\alpha \cancel{a} h_1^p + \beta \cancel{a} h_2^p = 0 \Leftrightarrow \alpha h_1^p + (1-\alpha) h_2^p = 0$$

$$\alpha = \frac{-h_2^p}{h_1^p - h_2^p}$$

Richardson Extrapolation: Observations,

What are α and β for a first-order (e.g. finite-difference) method if we choose $h_2 = h_1/2$?

$p=1$

$h=1$

$h=\frac{1}{2}$

$\alpha = \frac{-h_2}{h_1 - h_2} = \frac{-\frac{1}{2}}{1-\frac{1}{2}} = -1$

$\beta = 2$

$h=\frac{1}{4}$

$h=\frac{1}{8}$

Demo: Richardson with Finite Differences [cleared]

Outline

Introduction to Scientific Computing

Systems of Linear Equations

Linear Least Squares

Eigenvalue Problems

Nonlinear Equations

Optimization

Interpolation

Numerical Integration and Differentiation

Initial Value Problems for ODEs
- Existence, Uniqueness, Conditioning
- Numerical Methods (I)
- Accuracy and Stability
- Stiffness
- Numerical Methods (II)

Boundary Value Problems for ODEs

Partial Differential Equations and Sparse Linear Algebra

Fast Fourier Transform

Additional Topics

What can we solve already?

- Linear Systems: yes
- Nonlinear systems: yes
- Systems with derivatives: no

Some Applications

IVPs	BVPs
▶ Population dynamics $y_1' = y_1(\alpha_1 - \beta_1 y_2)$ (prey) $y_2' = y_2(-\alpha_2 + \beta_2 y_1)$ (predator) ▶ chemical reactions ▶ equations of motion	▶ bridge load ▶ pollutant concentration (steady state) ▶ temperature (steady state) ▶ waves (time-harmonic)

Demo: Predator-Prey System [cleared]

Initial Value Problems: Problem Statement

Want: Function $\boldsymbol{y} : [0, T] \to \mathbb{R}^n$ so that

- $\boldsymbol{y}^{(k)}(t) = \boldsymbol{f}(t, \boldsymbol{y}, \boldsymbol{y}', \boldsymbol{y}'', \dots, \boldsymbol{y}^{(k-1)})$ (*explicit*), or
- $\boldsymbol{f}(t, \boldsymbol{y}, \boldsymbol{y}', \boldsymbol{y}'', \dots, \boldsymbol{y}^{(k)}) = 0$ (*implicit*)

are called explicit/implicit *kth-order ordinary differential equations* (*ODEs*). Give a simple example.

$y' = \alpha y$ $\qquad$ $y(t) = \underline{\quad} e^{\alpha t}$

Not uniquely solvable on its own. What else is needed?

initial condition

need k ICs (initial conditions)

$y(0) = \dots$

$\vdots$

$y^{(k-1)}(0) = \dots$

IVP initial value problem

Reducing ODEs to First-Order Form

$y' = \ldots$

A kth order ODE can always be reduced to first order. Do this in this example:

$$y''(t) = f(y)$$

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}'(t) = \begin{bmatrix} y_2(t) \\ f(y_1(t)) \end{bmatrix} \leftarrow \text{reduced to first-order!}$$

$$y_1''(t) = (y_1'(t))' = (y_2(t))' = f(y_1(t))$$

May assume that ODE has been rewritten to first-order form.

Properties of ODEs

$$\vec{y}'(t) = f(t, \vec{y})$$

What is a linear ODE?

$$f(t, \vec{y}) = A(t)\vec{y} + \vec{b}(t)$$

What is a linear and homogeneous ODE?

$$f(t, \vec{y}) = A(t)\vec{y}$$

What is a constant-coefficient ODE?

$$f(t, \vec{y}) = A \quad \vec{y}$$

Properties of ODEs (II)

$$y'(t) = f(t, y)$$

What is an autonomous ODE?

$$\left.\begin{aligned} y_{n+1}'(t) &= 1 \\ y_{n+1}(t_0) &= t_0 \end{aligned}\right\} \quad y_{n+1}(t) = t$$

↳ May assume the ODE is autonomous

$$y'(t) = f(y(t))$$

Existence and Uniqueness

Consider the perturbed problem

$$\begin{cases} \boldsymbol{y}'(t) = \boldsymbol{f}(\boldsymbol{y}) \\ \boldsymbol{y}(t_0) = \boldsymbol{y}_0 \end{cases} \qquad \begin{cases} \widehat{\boldsymbol{y}}'(t) = \boldsymbol{f}(\widehat{\boldsymbol{y}}) \\ \widehat{\boldsymbol{y}}(t_0) = \widehat{\boldsymbol{y}}_0 \end{cases}$$

Then if $\boldsymbol{f}$ is *Lipschitz continuous* (has 'bounded slope'), i.e.

$$\|\boldsymbol{f}(\boldsymbol{y}) - \boldsymbol{f}(\widehat{\boldsymbol{y}})\| \leq L \, \|\boldsymbol{y} - \widehat{\boldsymbol{y}}\| \, ,$$

there exists a unique solution

What does this mean for uniqueness?

Conditioning

Unfortunate terminology accident: "Stability" in ODE-speak

To adapt to conventional terminology, we will use 'Stability' for

- the conditioning of the IVP, *and*
- the stability of the methods we cook up.

Some terminology:

An IVP is stable if and only if...

the solution at all times depends continuously on the IC

For all $\varepsilon > 0$ there exists a $\delta > 0$

$$\|\hat{y}_0 - y_0\| < \delta \Rightarrow \|y(t) - \hat{y}(t)\| < \varepsilon \text{ for all } t.$$

An IVP is asymptotically stable if and only if

$$\|\hat{y}(t) - y(t)\| \to 0$$

Example I: Scalar, Constant-Coefficient

e^{ibt}

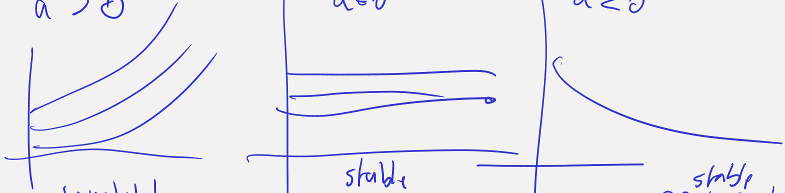
$$\begin{cases} y'(t) = \lambda y \\ y(0) = y_0 \end{cases} \quad \text{where} \quad \lambda = a + ib$$

Solution?

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

When is this stable?

$\mathrm{Re}(\lambda) > 0$, $a > 0$ | $= 0$, $a = 0$ | < 0, $a < 0$



unstable | stable but not asymptotically stable | stable, asymp. stable

Example II: Constant-Coefficient System

$$\begin{cases} \boldsymbol{y}'(t) = A\boldsymbol{y}(t) \\ \boldsymbol{y}(t_0) = \boldsymbol{y}_0 \end{cases}$$

Assume $V^{-1}\,\mathrm{AV} = D = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ diagonal. Find a solution.

$\vec{w}(t) = V^{-1}\vec{y}(t)$

$\vec{w}'(t) = V^{-1}\vec{y}'(t) = V^{-1}A\vec{y}(t) = V^{-1}AV\vec{w}(t)$

$= D\vec{w}(t)$

When is this stable?

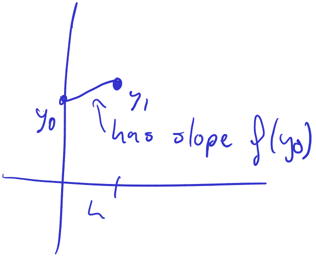
$\vec{w}' = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}\vec{w}$

If $\mathrm{Re}(\lambda_i) < 0$.

Euler's Method

Discretize the IVP

$$\begin{cases} \boldsymbol{y}'(t) = \boldsymbol{f}(\boldsymbol{y}) \\ \boldsymbol{y}(t_0) = \boldsymbol{y}_0 \end{cases}$$



- Discrete times: $t_1, t_2, \ldots$, with $t_{i+1} = t_i + h$
- Discrete function values: $\boldsymbol{y}_k \approx \boldsymbol{y}(t_k)$.

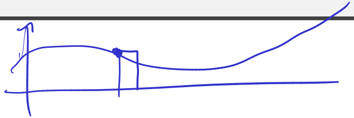
$\vec{y}_0$

$\vec{y}_1 = \vec{y}_0 + h \vec{f}(\vec{y}_0)$

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

A different interpretation:

$$y_k = y_{k-1} + \int_{t_{k-1}}^{t_k} f(y(\tau))\, d\tau$$



left rectangle rule

Euler's method: Forward and Backward

$$\boldsymbol{y}(t) = \boldsymbol{y}_0 + \int_{t_0}^{t} \boldsymbol{f}(\boldsymbol{y}(\tau))\mathrm{d}\tau,$$

Use 'left rectangle rule' on integral:

$$y_k = y_{k-1} + h f(y_{k-1}) \quad \longleftarrow \quad \text{"explicit"}$$

(plug 'n' chug)

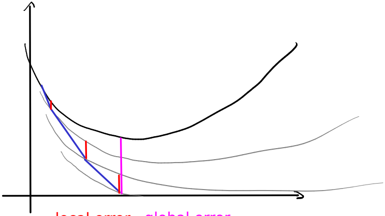
Use 'right rectangle rule' on integral:

$$y_k = y_{k-1} + h f(y_k) \quad \longleftarrow \quad \text{implicit}$$

(solve a nonlinear equation)

Demo: Forward Euler stability [cleared]

Global and Local Error



Let $u_k(t)$ be the function that solves the ODE with the initial condition $u_k(t_k) = y_k$. Define the local error at step k as...

Define the global error at step k as...

About Local and Global Error

Is global error $= \sum$local errors?

A time integrator is said to be *accurate of order p* if...

ODE IVP Solvers: Order of Accuracy

A time integrator is said to be *accurate of order p* if $\ell_k = O(h^{p+1})$

This requirement is one order higher than one might expect–why?

Stability of a Method

Find out when forward Euler is stable when applied to $y'(t) = \lambda y(t)$.

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

$$= \underbrace{(1+h\lambda)}_{|\cdot|<1} y_{k-1}$$

stable if $|1+h\lambda| < 1$

stability region of this method

Stability: Systems

What about stability for systems, i.e.

$$\boldsymbol{y}'(t) = A\boldsymbol{y}(t)?$$