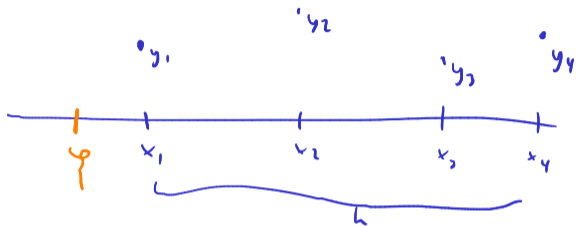


- EC HW 14 out later today



$$f'(a) \approx \alpha_1 y_1 + \alpha_2 y_2 + \alpha_3 y_3 + \alpha_4 y_4 + O(h^?)$$

$$\alpha_i = \psi_i(x_1, \dots, x_4)$$

# Differentiation Matrices

How can numerical differentiation be cast as a matrix-vector operation?

$$p_{r-1}(x) = \sum_{\alpha=1}^n \alpha_i \varphi_i(x)$$
$$p'_{r-1}(x) = \sum_{\alpha=1}^n \alpha_i \varphi'_i(x)$$
$$V' = \begin{pmatrix} \varphi'_1(x_1) & \varphi'_2(x_1) & \dots \\ \varphi'_1(x_2) & & \end{pmatrix}$$
$$V \vec{\alpha} = \vec{y} \Leftrightarrow \vec{\alpha} = V^{-1} \vec{y}$$
$$f'(\vec{x}) \approx \underbrace{D}_{V' V^{-1}} \underbrace{f(\vec{x})}_{\vec{y}}$$

Demo: Taking Derivatives with Vandermonde Matrices [cleared] (Build  $D$ )

$$\begin{pmatrix} f'(x_1) \\ \vdots \\ f'(x_n) \end{pmatrix} = \begin{matrix} \square \\ \text{D} \\ \square \\ \hline V'V^{-1} \end{matrix} \begin{pmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{pmatrix}$$

$$f'(y) \approx \alpha_1 y_1 + \alpha_2 y_2 + \alpha_3 y_3 + \alpha_4 y_4 + O(h^2)$$

$\Rightarrow$  Each row of  $D$  contains a finite difference rule

$$f'(x_i) \approx d_{i1} f(x_1) + \dots + d_{in} f(x_n)$$

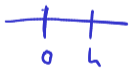


Shift:



→ does not change  $D$ , does not obey  $\neq D$  rule

Scale:



$$f'(0) \approx -\frac{1}{h} f(0) + \frac{1}{h} f(h)$$

$$= \frac{f(h) - f(0)}{h}$$

→ scaling nodes by  $\delta$ : become  $\frac{dx}{\delta}$

## Properties of Differentiation Matrices

How do I find second derivatives?

Does  $D$  have a nullspace?

## Numerical Differentiation: Shift and Scale

Does  $D$  change if we shift the nodes  $(x_i)_{i=1}^n \rightarrow (x_i + c)_{i=1}^n$ ?

Does  $D$  change if we scale the nodes  $(x_i)_{i=1}^n \rightarrow (\alpha x_i)_{i=1}^n$ ?

## Finite Difference Formulas from Diff. Matrices

How do the rows of a differentiation matrix relate to FD formulas?



Assume a large equispaced grid and 3 nodes w/same spacing. How to use?



## Finite Differences: via Taylor

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} + O(h^1)$$

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

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



## More Finite Difference Rules

Similarly:

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

(Centered differences)

Can also take higher order derivatives:  $\rightarrow$  using deriv. matrices:  $D^2$

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

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]

# 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

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}: [0, \infty) \rightarrow \mathbb{R}^2$$



IVPs	BVPs
<ul style="list-style-type: none"><li>▶ Population dynamics <math>y_1' = y_1(\alpha_1 - \beta_1 y_2)</math> (prey) <math>y_2' = y_2(-\alpha_2 + \beta_2 y_1)</math> (predator)</li><li>▶ chemical reactions</li><li>▶ equations of motion</li></ul>	<ul style="list-style-type: none"><li>▶ bridge load </li><li>▶ pollutant concentration (steady state)</li><li>▶ temperature (steady state)</li><li>▶ waves (time-harmonic)</li></ul>

Demo: Predator-Prey System [cleared]

## Initial Value Problems: Problem Statement

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

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

are called explicit/implicit  $k$ th-order ordinary differential equations (ODEs).

Give a simple example.

$$y' = \alpha y$$

$$y(t) = c \cdot e^{\alpha t}$$

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

$$y'' = f(t, y, y') \rightarrow \text{needs } y \text{ and } y'$$

$$\left. \begin{array}{l} \text{need } y(0) = \dots \\ \vdots \\ y^{(k-1)}(0) = \dots \end{array} \right\} k \text{ initial conditions}$$

## Reducing ODEs to First-Order Form

$$\vec{w}' = f(\vec{w})$$

A  $k$ th order ODE can always be reduced to first order. Do this in this example:

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

$$\begin{cases} w_1 = y \\ w_2 = y' \end{cases}$$

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix}' = \begin{bmatrix} w_2 \\ f(w_1) \end{bmatrix}$$

→ For numerics: need only worry about (systems of) first-order ODEs

## Properties of ODEs

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

What is a **linear** ODE?

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

What is a **linear and homogeneous** ODE?

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

What is a **constant-coefficient** ODE?

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

## Existence and Uniqueness

Consider the perturbed problem

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

$$\begin{aligned} y' &= \alpha y && \nearrow e^{\alpha y} \\ f(y) &= \alpha y \\ f'(y) &= \alpha \end{aligned}$$

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

$$\|\mathbf{f}(\mathbf{y}) - \mathbf{f}(\hat{\mathbf{y}})\| \leq L \|\mathbf{y} - \hat{\mathbf{y}}\|$$

(where  $L$  is called the *Lipschitz constant*), then...

- there exists a solution  $\mathbf{y}$  in a neighborhood of  $\mathbf{y}_0$
- $\|\vec{y}(t) - \vec{\hat{y}}(t)\| \leq e^{L(t-t_0)} \|\vec{y}_0 - \vec{\hat{y}}_0\|$

What does this mean for uniqueness?

Picard-Lindelöf theorem

Implicitly covers uniqueness, as well  
 $\vec{y}_0 = \vec{\hat{y}}_0 \Rightarrow \vec{y}(t) = \vec{\hat{y}}(t)$



## 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 ~~ODE~~ is **stable** if and only if...

IVP

The solution is continuously dependent on the IC.

For all  $\epsilon > 0$  there exists a  $\delta > 0$  so that

$$\| \vec{y}_0 - \vec{y}_0 \| < \delta \Rightarrow \| \vec{y}(t) - \vec{y}(t) \| < \epsilon \text{ for all } t \geq t_0.$$

An ~~ODE~~ is **asymptotically stable** if and only if

IVP

$$\| \vec{y}(t) - \vec{y}(t) \| \rightarrow 0 \quad t \rightarrow \infty$$

# Example I: Scalar, Constant-Coefficient

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

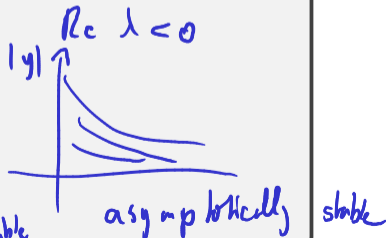
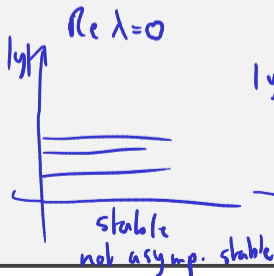
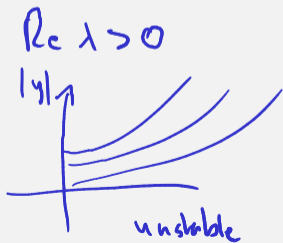
Solution?

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

magnitude.

When is this stable?

$|e^{ibt}| \leq 1$  "oscillation"



## Example II: Constant-Coefficient System

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

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

hom. const. coeff.

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

$$\vec{w} = V^{-1} \vec{y} \quad \leadsto \quad V \vec{w} = \vec{y}$$

$$w' = V^{-1} y' = V^{-1} A y = \cancel{V^{-1} V} D V^{-1} y = D w$$

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}' = \begin{pmatrix} 12 & \\ & 34 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

$$\begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}' = \begin{pmatrix} d_{11} w_1 \\ \vdots \\ d_{nn} w_n \end{pmatrix}$$

When is this stable?

$$\text{Re}(\lambda_i) < 0 \rightarrow \text{asympt. stable}$$

$> 0 \rightarrow$  unstable.

# Euler's Method

Discretize the IVP

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

← diff eq

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

← int eq.

$$\vec{y}(t) = \vec{y}_0 + \int_{t_0}^t \mathbf{f}(\mathbf{y}(\tau)) d\tau$$

Picard's int. eq.



use quadrature.

$$\text{Forward Euler } \mathbf{y}(t) = \mathbf{y}_0 + \mathbf{f}(\mathbf{y}_0) \cdot \Delta t$$

$$\text{"left rectangle rule": } \int_a^b f(x) dx \approx f(a) \cdot (b-a)$$

## Euler's method: Forward and Backward

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

Use 'left rectangle rule' on integral:

$$\vec{y}_{k+1} = \vec{y}_k + h f(\vec{y}_k)$$

explicit  $\rightarrow$  can just evaluate  $y_{k+1}$

Use 'right rectangle rule' on integral:

$$\vec{y}_{k+1} = \vec{y}_k + h f(\vec{y}_{k+1})$$

implicit  $\rightarrow$  solve for  $y_{k+1}$

Demo: Forward Euler stability [cleared]