Object-oriented scientific computing

Pras Pathmanathan

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Introduction

For various types of differential equation, we will:

1. Discuss **numerical schemes** that can be used for the equations, and summarise some of the important features
2. Discuss a sensible **object-oriented design** to implement the scheme
3. Introduce a **real-world use**

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Object Oriented Programming

Classes

The basic data-types in standard programming are integers, floating point real numbers, boolean flags, etc, and arrays (vectors) of these.

Object-oriented programming is based on **user-defined complex data-types**, known as **classes**, representing, for example: Mesh, Cat, Measurement, PdeSolver, ..

Classes are composed of **data** (**member variables**) and **methods** (functions)

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Classes - example

For example, consider the following simple class for representing a 'human'

```
class Human:
    Data:
        mAge (an integer)
    Methods:
        SetAge(age)
        GetAge()
```

The usage could be something like

```
Human james;
james.SetAge(22);

Human miguel;
..
if (james.GetAge() < miguel.GetAge())
  ..
```

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```

Classes - motivation

This is in contrast to, for example (using Matlab-style code):

```
james_age = 22;
miguel_age = 24;
..
if james_age < miguel_age
  ..
```

or something like

```
names = ['james','miguel'];
ages = [22, 24];
..
```

This gets messy if we now have to also store heights, weights, etc

Classes - inheritance

Suppose we want to write a class for an 'academic'. We don't want to have to copy all the code relating to the fact that academics are (usually) humans.

Inheritance gets around this

```
class Academic inherits from Human:
    Data:
        mNumPapers
    Methods:
        PublishPaper()          (increments mNumPapers by one)
        GetNumPapers()
```

Classes - inheritance

Example usage:

```
Academic hawking;
..
if (hawking.GetAge()<30 && hawking.GetNumPapers()>30)
  ..
```

- The original class (`Human`) is referred to as the parent class / superclass / base class
- The inheriting class (`Academic`) is referred to as the child class / subclass / derived class.

Classes - private/public data

`class Academic` *inherits from* `Human`:

Data:

`mNumPapers`

Methods:

`PublishPaper()` *(increments* `mNumPapers` *by one)*

`GetNumPapers()`

Data (and methods) can be declared to be **private** or **public**. If `mNumPapers` is declared as private:

```
Acamedic newton;
newton.mNumPapers = 35;
```

would not be allowed.

Classes - security

If `mNumPapers` is private, compare the security of

```
class Academic inherits from Human:
    Data:
        mNumPapers                          (initialised to zero)
    Methods:
        PublishPaper()                      (increments mNumPapers by one)
        GetNumPapers()
```

with

```
Academic hawking
Academic newton
newton.PublishPaper()
```

versus

```
hawking_num_papers = 0;
newton_num_papers = 1;
```

Abstract classes

Abstract classes are classes that contain an abstract (or 'pure virtual') method. These are methods which are declared but not implemented.

```
class AbstractAnimal:
    Data:
        mIsHungry
    Methods:
        Eat()                                   (set mIsHungry to false)
        MakeNoise()          (Abstract method, ie implementation not given)
```

Abstract classes **cannot be instantiated**, i.e. the following is not allowed

```
AbstractAnimal rover
```

Instead, a subclass must be written which implements the abstract method..

Abstract classes

Example 'concrete classes', inheriting from `AbstractAnimal`:

```
class Dog inherits from AbstractAnimal:
    Methods:
        MakeNoise()                                   (print out 'woof')
```

```
class Cat inherits from AbstractAnimal:
    Methods:
        MakeNoise()                                   (print out 'meow')
```

As these have implemented the abstract methods, they can be instantiated:

```
Cat scratchy;
Dog brian;
scratchy.MakeNoise();
brian.MakeNoise();
```

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    Methods:
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class Cat inherits from AbstractAnimal:
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        MakeNoise()                                   (print out 'meow')
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As these have implemented the abstract methods, they can be instantiated:

```
Cat scratchy;
Dog brian;
scratchy.MakeNoise();
brian.MakeNoise();
```

Abstract classes

Consider the following:

```
class Human:
    Methods:
        ..
        SetPet(abstractAnimal)
```

The code inside `SetPet()` doesn't know anything about what animals exist, but can still call `MakeNoise()`.

Colour scheme

`AbstractAnimal`:
Member var: `mIsHungry`
Method: `Eat()`
Abs. method: `MakeNoise()`

`Dog`: *inherits from* `AbstractAnimal`
Implemented method: `MakeNoise()`

`Cat`: *inherits from* `AbstractAnimal`
Implemented method: `MakeNoise()`

Solving ODEs

The forward and backward Euler methods

Consider the system of ODEs:

$$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} = f(t, \mathbf{y})$$

with initial condition $\mathbf{y}(0) = \mathbf{y}_0$. Given a timestep Δt, we require a numerical approximation $\mathbf{y}^0 (= \mathbf{y}_0), \mathbf{y}^1, \mathbf{y}^2, \ldots$ Here $\mathbf{y}^n$ represents the numerical solution at time $t^n = n\Delta t$.

The **forward Euler discretisation** is

$$\frac{\mathbf{y}^{n+1} - \mathbf{y}^n}{\Delta t} = f(t^n, \mathbf{y}^n) \qquad \Rightarrow \qquad \mathbf{y}^{n+1} = \mathbf{y}^n + \Delta t\, f(t^n, \mathbf{y}^n)$$

which explicitly gives each $\mathbf{y}^{n+1}$ in terms of $\mathbf{y}^n$, i.e. this is an **explicit** scheme.

The **backward Euler discretisation** is

$$\frac{\mathbf{y}^{n+1} - \mathbf{y}^n}{\Delta t} = f(t^{n+1}, \mathbf{y}^{n+1}) \qquad \Rightarrow \qquad \mathbf{y}^{n+1} - \Delta t\, f(t^{n+1}, \mathbf{y}^{n+1}) = \mathbf{y}^n$$

which in general is a nonlinear system of equations for $\mathbf{y}^{n+1}$, i.e. an **implicit** scheme.

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Multi-step methods

We could also use the computed solution at previous timesteps.

Let f^n represent $f(t^n, y^n)$. The **Adams-Bashforth method** is

$$y^{n+2} = y^{n+1} + \frac{1}{2}\Delta t \left(3f^{n+1} - f^n\right)$$

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Accuracy

Write an explicit one-step method as: $y^{n+1} = y^n + \Delta t\, \phi(t^n, y^n; \Delta t)$

Truncation error

The truncation error is defined as

$$T^n = y(t^{n+1}) - y(t^n) - \Delta t\, \phi(t^n, y(t^n); \Delta t);$$

or, equivalently: **if** $y(t^n) = y^n$, then

$$T^n = y(t^{n+1}) - y^{n+1}$$

i.e. it is the local error induced in a single timestep. Note:

- for implicit/multi-step methods there is an analogous definition.
- some definitions divide through by Δt

It is easy to show using a Taylor expansion that

$$T^n = \mathcal{O}(\Delta t^2)$$

for both forward and backward Euler.

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Accuracy

Global error

The global error is simply defined as

$$e_n = y(t^n) - y^n$$

We only consider global error on some fixed time interval $[0, T_{\text{end}}]$. Let $T_{\text{end}} = N\Delta t$, i.e. let N be the total number timesteps taken.

For the Euler methods we expect $e_N = \mathcal{O}(N\Delta t^2) = \mathcal{O}(T_{\text{end}}\Delta t) = \mathcal{O}(\Delta t)$, and therefore that $e_n = \mathcal{O}(\Delta t)$.

This can be shown to be the case under assuming mild conditions[1] on f:

$$e_n = \mathcal{O}(\Delta t)$$

We say the forward and backward Euler methods are **first-order**

[1] Basically, $f(t, y)$ is Lipschitz continuous in y—the same conditions which are required for the existence of a unique solution of the ODE $\frac{dy}{dt} = f(t, y)$

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Stability

There are various notions of stability

Zero-stability

- Zero stability is the stability of the numerical solution to changes in initial condition y^0
- This is the essentially that small errors (at any time) do not grow unbounded
- A non-zero-stable method would be useless computationally
- **Dahlquist equivalence theorem**: for a 'consistent' multistep method with 'consistent' initial values: zero-stability $\Leftrightarrow$ convergence

A-stability

Consider the ODE

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \lambda y, \text{ with } y(0) = 1 \qquad \Rightarrow \qquad y = e^{\lambda t}$$

If $\lambda < 0$, then $y \to 0$ as $t \to \infty$.

Does the numerical solution y^n satisfy $y^n \to 0$ as $n \to \infty$, with fixed Δt?

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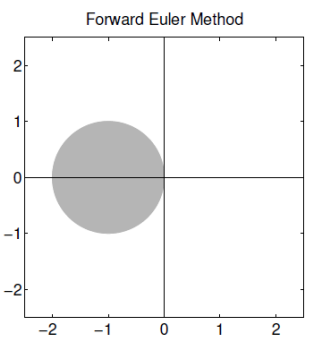
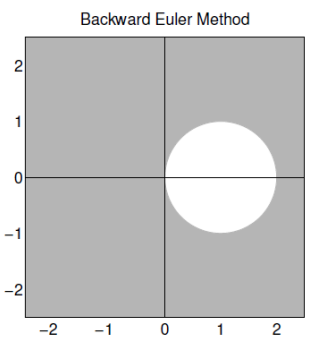
Does the numerical solution y^n satisfy $y^n \to 0$ as $n \to \infty$, with fixed Δt?

If $\lambda < 0$

- Forward Euler: $y^n \to 0$ only if $\Delta t < -\frac{2}{\lambda}$, i.e. conditional stability
- Backward Euler: $y^n \to 0$ for all Δt, i.e. unconditional stability





Other discretisations

One-step:

- **Forward Euler**: $y^{n+1} = y^n + \Delta t\, f(t^n, y^n)$ $\mathcal{O}(\Delta t)$
- **Backward Euler**: $y^{n+1} = y^n + \Delta t\, f(t^{n+1}, y^{n+1})$ $\mathcal{O}(\Delta t)$
- **Trapezoidal rule**: $y^{n+1} = y^n + \frac{1}{2}\Delta t \left(f(t^n, y^n) + f(t^{n+1}, y^{n+1})\right)$ $\mathcal{O}(\Delta t^2)$
- **Heun's method**:
  $y^{n+1} = y^n + \frac{1}{2}\Delta t \left(f(t^n, y^n) + f(t^{n+1}, y^n + \Delta t\, f(t^n, y^n))\right)$ $\mathcal{O}(\Delta t^2)$
- **Four-stage Runge-Kutta**:
  $y^{n+1} = y^n + \frac{1}{6}\Delta t(k_1 + 2k_2 + 2k_3 + k_4)$ $\mathcal{O}(\Delta t^4)$
  where $k_1 = f(t^n, y^n)$, $k_2 = f(t^n + \frac{1}{2}\Delta t, y^n + \frac{1}{2}\Delta t\, k_1)$,...

Multi-step:

- **Simpson's Rule**: $y^{n+2} = y^{n+1} + \frac{1}{3}\Delta t \left(f^{n+2} + 4f^{n+1} + f^n\right)$ $\mathcal{O}(\Delta t^4)$
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- **Four-stage Runge-Kutta**:
  $y^{n+1} = y^n + \frac{1}{6}\Delta t(k_1 + 2k_2 + 2k_3 + k_4)$ $\mathcal{O}(\Delta t^4)$
  where $k_1 = f(t^n, y^n)$, $k_2 = f(t^n + \frac{1}{2}\Delta t, y^n + \frac{1}{2}\Delta t\, k_1)$,...

Multi-step:

- **Simpson's Rule**: $y^{n+2} = y^{n+1} + \frac{1}{3}\Delta t \left(f^{n+2} + 4f^{n+1} + f^n\right)$ $\mathcal{O}(\Delta t^4)$
- **Adams-Bashforth**: $y^{n+2} = y^{n+1} + \frac{1}{2}\Delta t \left(3f^{n+1} - f^n\right)$ $\mathcal{O}(\Delta t^2)$

Other discretisations

One-step:

- **Forward Euler**: $y^{n+1} = y^n + \Delta t\, f(t^n, y^n)$ $\mathcal{O}(\Delta t)$
- **Backward Euler**: $y^{n+1} = y^n + \Delta t\, f(t^{n+1}, y^{n+1})$ $\mathcal{O}(\Delta t)$
- **Trapezoidal rule**: $y^{n+1} = y^n + \frac{1}{2}\Delta t \left(f(t^n, y^n) + f(t^{n+1}, y^{n+1})\right)$ $\mathcal{O}(\Delta t^2)$
- **Heun's method**:
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Object-oriented implementation

A (standard) Matlab approach uses function pointers:

```
[T,Y] = ode45(@my_func,[0 1],[1 2 3]);

function dydt = my_func(t,y)
dydt = y.^2;
```

Object-oriented approach:

`AbstractOdeSystem`:

Member var: `mSize`

▷ *i.e. the dimension of the vector* $\mathbf{y}$

Abs. method: `EvaluateYDerivatives(t, y)`

▷ *Declares the function representing* $f(t, \mathbf{y})$

`MyOdeSystem`: *inherits from* `AbstractOdeSystem`

Implemented method: `EvaluateYDerivatives(t, y)`

▷ *One particular choice of* $f(t, \mathbf{y})$

Object-oriented implementation: solvers

`AbstractOneStepOdeSolver`:

Abs. method: `Solve(abstractOdeSystem,t0,t1,initialCond)`

`ForwardEulerSolver`: *inherits from* `AbstractOneStepOdeSolver`

Implemented method: `Solve(..)`

- ▷ *Implements a forward Euler solve*

`BackwardEulerSolver`: *inherits from* `AbstractOneStepOdeSolver`

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This isn't optimal, because the loop over time is implemented in both the solvers, but isn't specific to either

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Object-oriented implementation: solvers

`AbstractOneStepOdeSolver`:

Method: `Solve(abstractOdeSystem,t0,t1,initialCond)`

▷ *Implements a loop over time, and each timestep calls the following:*

Abs. method: `CalculateNextYValue(currentYValue)`

`ForwardEulerSolver`: *inherits from* `AbstractOneStepOdeSolver`

Implemented method: `CalculateNextYValue(..)`

▷ *Takes in* $\mathbf{y}^n$, *returns* $\mathbf{y}^{n+1} = \mathbf{y}^n + \Delta t\, f(t^n, \mathbf{y}^n)$

`BackwardEulerSolver`: *inherits from* `AbstractOneStepOdeSolver`

Implemented method: `CalculateNextYValue(..)`

▷ *Takes in* $\mathbf{y}^n$, *solves* $\mathbf{y}^{n+1} - \Delta t\, f(t^{n+1}, \mathbf{y}^{n+1}) = \mathbf{y}^n$, *returns* $\mathbf{y}^{n+1}$

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