Final project worth 30% of grade
Due on Monday December 18th at 5 PM on Canvas, along with associated code
In general, should be completed in teams of two or three.
Single-person projects will be allowed with instructor permission. $n \geq 4$ person projects will be allowed with instructor permission and a written statement detailing the division of the work.
Piazza is best place to find teammates
Very rough length guidelines

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- Precise length of write-up is not important. Scientific content is more important.
- Optional: submit a poster to the CS fall poster session. IACS will cover poster cost. Roughly count as 25% reduction in write-up length.
Find an application area of interest and apply methods from the course to it.

Project must involve some coding. No purely theoretical projects allowed.

Fine to take problems directly from research, within reason. It should be an aspect of a project that is carried out for this course, as opposed to something already ongoing.
By November 16th at 6 PM, each team should arrange a half-hour meeting with Chris or the TFs to discuss a project idea and direction.

Four points automatically awarded for doing this.

Nothing written is necessary—only the meeting is required. However, feel free to bring documents, papers, or other resources to the meeting.

Total grade for project: 60 points. A detailed breakdown is posted on the website.
Finite Difference Approximations

Given a function $f : \mathbb{R} \to \mathbb{R}$

We want to approximate derivatives of $f$ via simple expressions involving samples of $f$

As we saw in Unit 0, convenient starting point is Taylor’s theorem

$$f(x + h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \cdots$$
Solving for $f'(x)$ we get the \textbf{forward difference formula}

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

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

Here we neglected an $O(h)$ term
Similarly, we have the Taylor series

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

which yields the backward difference formula

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

Again we neglected an \( O(h) \) term
Finite Difference Approximations

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

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

$$\approx \frac{f(x + h) - f(x - h)}{2h}$$

In this case we neglected an $O(h^2)$ term
Finite Difference Approximations

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

$$f''(x) = \frac{f(x + h) - 2f(x) + f(x - h)}{h^2} - \frac{f^{(4)}(x)}{12}h^2 + \ldots$$

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

Again we neglected an $O(h^2)$ term
Finite Difference Stencils

Forward diff. 

Backward diff. 

Centered diff. 
$1^{st}$ derivative 

Centered diff. 
$2^{nd}$ derivative
Finite Difference Approximations

We can use Taylor expansion to derive approximations with higher order accuracy, or for higher derivatives.

This involves developing F.D. formulae with “wider stencils,” i.e. based on samples at $x \pm 2h, x \pm 3h, \ldots$

But there is an alternative that generalizes more easily to higher order formulae:

Differentiate the interpolant!
Finite Difference Approximations

Linear interpolant at \( \{(x_0, f(x_0)), (x_0 + h, f(x_0 + h))\} \) is

\[
p_1(x) = f(x_0) \frac{x_0 + h - x}{h} + f(x_0 + h) \frac{x - x_0}{h}
\]

Differentiating \( p_1 \) gives

\[
p'_1(x) = \frac{f(x_0 + h) - f(x_0)}{h},
\]

which is the forward difference formula

**Question:** How would we derive the backward difference formula based on interpolation?
Similarly, quadratic interpolant, $p_2$, from interpolation points \( \{ x_0, x_1, x_2 \} \) yields the centered difference formula for $f'$ at $x_1$:

- Differentiate $p_2(x)$ to get a linear polynomial, $p'_2(x)$
- Evaluate $p'_2(x_1)$ to get centered difference formula for $f'$

Also, $p''_2(x)$ gives the centered difference formula for $f''$

Note: Can apply this approach to higher degree interpolants, and interp. pts. need not be evenly spaced
So far we have talked about finite difference formulae to approximate $f'(x_i)$ at some specific point $x_i$.

**Question:** What if we want to approximate $f'(x)$ on an interval $x \in [a, b]$?

**Answer:** We need to simultaneously approximate $f'(x_i)$ for $x_i$, $i = 1, \ldots, n$. 
Differentiation Matrices

We need a map from the vector \( F \equiv [f(x_1), f(x_2), \ldots, f(x_n)] \in \mathbb{R}^n \) to the vector of derivatives \( F' \equiv [f'(x_1), f'(x_2), \ldots, f'(x_n)] \in \mathbb{R}^n \).

Let \( \tilde{F}' \) denote our finite difference approximation to the vector of derivatives, *i.e.* \( \tilde{F}' \approx F' \).

Differentiation is a linear operator\(^1\), hence we expect the map from \( F \) to \( \tilde{F}' \) to be an \( n \times n \) matrix.

This is indeed the case, and this map is a **differentiation matrix**, \( D \).

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\(^1\)Since \( (\alpha f + \beta g)' = \alpha f' + \beta g' \)
Differentiation Matrices

Row $i$ of $D$ corresponds to the finite difference formula for $f'(x_i)$, since then $D_{(i,:)} F \approx f'(x_i)$

e.g. for forward difference approx. of $f'$, non-zero entries of row $i$ are

$$D_{ii} = -\frac{1}{h}, \quad D_{i,i+1} = \frac{1}{h}$$

This is a sparse matrix with two non-zero diagonals
Differentiation Matrices

\begin{align*}
n &= 100 \\
h &= 1/(n-1) \\
D &= \text{np.diag}(-\text{np.ones}(n)/h) + \text{np.diag}(\text{np.ones}(n-1)/h, 1) \\
\text{plt.spy}(D) \\
\text{plt.show}()
\end{align*}
Differentiation Matrices

But what about the last row?

\[ D_{n,n+1} = \frac{1}{h} \text{ is ignored!} \]
Differentiation Matrices

We can use the backward difference formula (which has the same order of accuracy) for row $n$ instead

$$D_{n,n-1} = -\frac{1}{h}, \quad D_{nn} = \frac{1}{h}$$
Integration of ODE Initial Value Problems

In this chapter we consider problems of the form

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

Here \( y(t) \in \mathbb{R}^n \) and \( f : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n \)

Writing this system out in full, we have:

\[
\begin{bmatrix}
  y'_1(t) \\
  y'_2(t) \\
    \vdots \\
  y'_n(t)
\end{bmatrix}
= \begin{bmatrix}
  f_1(t, y) \\
  f_2(t, y) \\
    \vdots \\
  f_n(t, y)
\end{bmatrix}
= f(t, y(t))
\]

This is a system of \( n \) coupled ODEs for the variables \( y_1, y_2, \ldots, y_n \)
ODE IVPs

Initial Value Problem implies that we know $y(0)$, i.e. $y(0) = y_0 \in \mathbb{R}^n$ is the initial condition.

The order of an ODE is the highest-order derivative that appears.

Hence $y'(t) = f(t, y)$ is a first order ODE system.
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:

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

Let \( v = y' \), then

\[ v'(t) = \frac{F(t, y, v)}{m} \]
\[ y'(t) = v(t) \]

and \( y(0) = y_0, v(0) = v_0 \)
ODE IVPs: A Predator–Prey ODE Model

For example, a two-variable nonlinear ODE, the Lotka–Volterra equation, can be used to model populations of two species:

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

The \( \alpha \) and \( \beta \) are modeling parameters, describe birth rates, death rates, predator-prey interactions.
Both Python and MATLAB have very good ODE IVP solvers

They employ adaptive time-stepping (\( h \) is varied during the calculation) to increase efficiency

Python has functions \texttt{odeint} (a general purpose routine) and \texttt{ode} (a routine with more options)

Most popular MATLAB function is \texttt{ode45}, which uses the classical fourth-order Runge–Kutta method

In the remainder of this chapter we will discuss the properties of methods like the Runge–Kutta method
Approximating an ODE IVP

Given $y' = f(t, y)$, $y(0) = y_0$: suppose we want to approximate $y$ at $t_k = kh$, $k = 1, 2, \ldots$

**Notation**: Let $y_k$ be our approx. to $y(t_k)$

**Euler’s method**: Use finite difference approx. for $y'$ and sample $f(t, y)$ at $t_k$:

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

Note that this, and all methods considered in this chapter, are written the same regardless of whether $y$ is a vector or a scalar.

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$^2$Note that we replace $y(t_k)$ by $y_k$
Euler’s Method

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

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

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

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

Again, this gives Euler’s method:

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

Python example: Euler’s method for $y' = \lambda y$
Backward Euler Method

We can derive other methods using the same quadrature-based approach.

Apply \( n = 0 \) Newton–Cotes quadrature based on interpolation point \( t_{k+1} \) to

\[
y(t_{k+1}) = y(t_k) + \int_{t_k}^{t_{k+1}} f(s, y(s))ds
\]

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 for \( y_{k+1} \) which requires some extra work

\[
y_{k+1} = y_k + hf(t_{k+1}, y_{k+1})
\]
Backward Euler Method

For example, approximate $y' = 2\sin(ty)$ using backward Euler:

At the first step ($k = 1$), we get

$$y_1 = y_0 + h\sin(t_1 y_1)$$

To compute $y_1$, let $F(y_1) \equiv y_1 - y_0 - h\sin(t_1 y_1)$ and solve for $F(y_1) = 0$ via, say, Newton’s method

Hence implicit methods are more complicated and more computationally expensive at each time step

Why bother with implicit methods? We’ll see why shortly...
Trapezoid Method

We can derive methods based on higher-order quadrature

Apply \( n = 1 \) Newton–Cotes quadrature (Trapezoid rule) at \( t_k \), \( t_{k+1} \) to

\[
y(t_{k+1}) = y(t_k) + \int_{t_k}^{t_{k+1}} f(s, y(s))\,ds
\]

to get the Trapezoid Method:

\[
y_{k+1} = y_k + \frac{h}{2} \left( f(t_k, y_k) + f(t_{k+1}, y_{k+1}) \right)
\]
One-Step Methods

The three methods we’ve considered so far have the form

\[ y_{k+1} = y_k + h\Phi(t_k, y_k; h) \]  \hspace{1cm} (explicit)

\[ y_{k+1} = y_k + h\Phi(t_{k+1}, y_{k+1}; h) \]  \hspace{1cm} (implicit)

\[ y_{k+1} = y_k + h\Phi(t_k, y_k, t_{k+1}, y_{k+1}; h) \]  \hspace{1cm} (implicit)

where the choice of the function \( \Phi \) determines our method.

These are called one-step methods: \( y_{k+1} \) depends on \( y_k \).

(One can also consider multistep methods, where \( y_{k+1} \) depends on earlier values \( y_{k-1}, y_{k-2}, \ldots \); we’ll discuss this briefly later.)
We now consider whether one-step methods converge to the exact solution as $h \to 0$.

Convergence is a crucial property, we want to be able to satisfy an accuracy tolerance by taking $h$ sufficiently small.

In general a method that isn’t convergent will give misleading results and is useless in practice!
Convergence

We define \textit{global error}, \( e_k \), as the total accumulated error at \( t = t_k \)

\[
e_k \equiv y(t_k) - y_k
\]

We define \textit{truncation error}, \( T_k \), as the amount “left over” at step \( k \) when we apply our method to the exact solution and divide by \( h \)

e.g. for an explicit one-step ODE approximation, we have

\[
T_k \equiv \frac{y(t_{k+1}) - y(t_k)}{h} - \Phi(t_k, y(t_k); h)
\]
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

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

Hence $hT_k$ is the error introduced in one step of our ODE approximation$^3$

Therefore the global error $e_k$ is determined by the accumulation of the $T_j$ for $j = 0, 1, \ldots, k - 1$

Now let’s consider the global error of the Euler method in detail.

$^3$Because of this fact, the truncation error is defined as $hT_k$ in some texts.
Convergence

**Theorem:** Suppose we apply Euler’s method for steps 1, 2, ..., $M$, to $y' = f(t, y)$, 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

$$|e_k| \leq \frac{(e^{L_f t_k} - 1)}{L_f} \left[ \max_{0 \leq j \leq k-1} |T_j| \right], \quad k = 0, 1, \ldots, M,$$

where $T_j$ is the Euler method truncation error.\(^4\)

\(^4\)Notation used here supposes that $y \in \mathbb{R}$, but the result generalizes naturally to $y \in \mathbb{R}^n$ for $n > 1$.\(^4\)
Convergence

Proof: From the definition of truncation error for Euler’s method 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

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

hence

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

Proof (continued...):

This gives a geometric progression, e.g. for \( k = 2 \) we have

\[
|e_3| \leq (1 + hL_f)|e_2| + h|T_2|
\]

\[
\leq (1 + hL_f)((1 + hL_f)|e_1| + h|T_1|) + h|T_2|
\]

\[
\leq (1 + hL_f)^2 h|T_0| + (1 + hL_f)h|T_1| + h|T_2|
\]

\[
\leq h \left[ \max_{0 \leq j \leq 2} |T_j| \right] \sum_{j=0}^{2} (1 + hL_f)^j
\]

Or, 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 (continued…):

Hence use the formula

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

with \( r \equiv (1 + hL_f) \), to get

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

Finally, we use the bound\(^5\) \( 1 + hL_f \leq \exp(hL_f) \) to get the desired result. \( \square \)

\(^5\)For \( x \geq 0, 1 + x \leq \exp(x) \) by power series expansion \( 1 + x + x^2/2 + \cdots \)
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:

\[
|f(t, u) - f(t, v)| = |f_y(t, \theta)||u - v|,
\]

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

Hence we can set:

\[
L_f = \max_{t \in [0, t_M]} \max_{\theta \in (u, v)} |f_y(t, \theta)|
\]
However, $f$ doesn’t have to be continuously differentiable to satisfy Lipschitz condition!

\[ |f(x) - f(y)| = |x - y|, \]  
\[ |f(x) - f(y)| = |x| - |y| \leq |x - y|, \]  
\[ L_f = 1 \]  
in this case

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\[ ^6 \text{This is the reverse triangle inequality} \]